

Numerical Study of Spin and Chiral Order in a Two-Dimensional XY Spin Glass

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The two-dimensional XY spin glass is studied numerically by a finite size defect energy scaling method at $T = 0$ in the vortex representation which allows us to compute the exact (in principle) spin and chiral domain wall energies. We confirm earlier predictions that there is no glass phase at any finite T . Our results strongly support the conjecture that both spin and chiral order have the same correlation length exponent $\nu_s = \nu_c \approx 2.70$. Preliminary results in 3D are also obtained. [S0031-9007(99)09184-X]

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The XY spin glass has been the subject of considerable attention and controversy for some time and is still not understood. It has been known since the seminal work of Villain [1] that vector spin glass models have chiral or reflection symmetry in addition to the continuous rotational symmetry. Consequently, the XY spin glass may have both spin glass and chiral glass orders. It is widely accepted that, in 2D and 3D, chiral and spin variables decouple at long distances and order independently [2–6] although there is a hint that this may not hold in 4D [7]. Numerical estimates of the correlation length exponents $\nu_{s,c}$ in 2D, when both spin (s) and chiral (c) order set in at $T = 0$ as $\xi_{s,c} \sim T^{-\nu_{s,c}}$, indicate that $\nu_c = 2.57 \pm 0.003$ and $\nu_s = 1.29 \pm 0.02$ [6] which agree with older, less accurate estimates [2,3,5,8]. These results seem to establish the decoupling of chiral and spin degrees of freedom, but analytic work on special models [9–11] implies that, for XY spin glasses below their lower critical dimension $d_l > 2$ when order sets in at $T = 0$, *both* correlation lengths diverge with the *same* exponent $\nu_s = \nu_c$. To add to the confusion, there is some evidence in 3D that chiral order sets in at $T > 0$ while spin glass order occurs only at $T = 0$ [2–4,12–14]. These numerical investigations have led to the accepted folklore that the lower critical dimension $d_l \geq 4$ for spin glass order [14,15]. A very recent simulation [6] concludes that earlier simulations are misleading because the spin defect energy begins to grow with system size L at values of L just beyond the limit accessible to earlier attempts and that $d_l < 3$. However, chiral order is robust in 3D. In 2D, all simulations agree that chiral and spin glass order set in at $T = 0$ but with different exponents $\nu_c \approx 2\nu_s \approx 2.6$.

The situation is very confused since, to our knowledge, there is no unambiguous proof of any of the folklore outlined above [16–18], numerical simulations are contradictory [6], and analytic work [9–11] contradicts the *apparently* unambiguous numerical simulations in 2D. In this Letter, we attempt to clarify the situation and our essential conclusion is that, by carefully defining spin and chiral defect energies, we find numerical agreement

with the conjecture [10] that $\theta_s = \theta_c < 0$ in 2D where $\theta_{s,c} = -1/\nu_{s,c}$ are the $T = 0$ stiffness exponents. In the absence of any rigorous testable results, this very plausible conjecture is the *only*, to our knowledge, analytic prediction existing and is the only check we have on the validity or otherwise of the numerical method used. If the conjecture is correct, a valid numerical simulation must agree with it and the implications go far beyond minor points such as the numerical values of stiffness exponents but implies that much of the XY spin glass folklore is incorrect. $2 < d_l < 3$ for *both* spin and chiral glass order, the chiral glass scenario $\theta_s < 0$ and $\theta_c > 0$ in 3D is not possible but both are positive and the presently accepted numerical values in 2D and 3D need reexamination.

A natural way to investigate order is to compute the domain wall, defect, or droplet energy $\Delta E(L)$ of a system of size L for several realizations of disorder (samples) for different values of L and fit to the finite size scaling ansatz [13,19,20] $\langle \Delta E(L) \rangle \sim L^{\theta_{s,c}}$. Here $\langle \dots \rangle$ denotes an average over disorder, $\Delta E(L) = E_D(L) - E_0(L)$ the defect energy with $E_0(L)$ the ground state (GS) energy, $E_D(L)$ the energy of the system containing a relative spin or chiral defect, and $\theta_{s,c}$ is the stiffness exponent. There are two main difficulties in applying these ideas to a finite disordered system. The first is how to define E_0 and E_D for a finite system with disorder since the GS configuration and energy depend on the imposed boundary conditions (BC). A spin or chiral defect is induced by an appropriate change in these BC and E_D is the minimum energy of the system subject to these new BC. The second is the computational problem of finding E_0 and E_D sufficiently accurate so the error in $\langle \Delta E(L) \rangle$ can be controlled and kept small. The numerical data are fitted to the scaling form in an attempt to verify the scaling ansatz and to obtain numerical values of the fundamental stiffness exponents $\theta_{s,c}$. The numerical constraints limit the accessible sizes L to very small values when the BC have large effects and it is essential to treat the BC properly to define E_0 and E_D consistently for a fit of the numerical data to a scaling form to have any meaning.

The Hamiltonian of a $\pm J$ XY spin glass on a $L \times L$ square lattice is

$$H = \sum_{\langle ij \rangle} V(\theta_i - \theta_j - A_{ij}), \quad (1)$$

where $V(\phi)$ is an even 2π periodic function of ϕ with a maximum at $\phi = \pi$, usually taken to be $V(\phi_{ij}) = -J_{ij} \cos(\phi_{ij})$ with the coupling $J_{ij} = J > 0$ for ij nearest neighbor sites of a square lattice. The random bond variables $A_{ij} = 0, \pi$ with equal probability $1/2$ correspond to ferro- and antiferromagnetic coupling between neighboring spins. We imagine the system of Eq. (1) on a torus which corresponds to imposing periodic BC on the phases $\theta_{i_x, i_y} = \theta_{i_x+L, i_y} = \theta_{i_x, i_y+L}$ with $i_{x,y} = 1, \dots, L$ and coupling spins on opposite faces by some interaction $\tilde{V}(\theta_{L, i_y}, \theta_{1, i_y})$ and $\tilde{V}(\theta_{i_x, L}, \theta_{i_x, 1})$ which define the BC. We define the GS by minimizing the energy with respect to the L^2 bulk variables θ_i and the form of \tilde{V} . Because of the symmetries of the XY spin glass [1], we restrict the form of \tilde{V} to those which can induce a spin or chiral defect. For a spin defect, $\tilde{V} = V(\theta_i - \theta_j - A_{ij})$ where the A_{ij} between corresponding sites i, j on opposite faces may be varied to find the minimum energy E_0 . It is not necessary to vary every A_{ij} as each elementary plaquette on the torus is equivalent and the plaquettes between opposite faces are indistinguishable from the others and play no special role. We therefore keep fixed the frustrations $f_{\mathbf{r}} = \sum_{\square_{\mathbf{r}}} A_{ij}/2\pi$ where the sum is over the bonds in a clockwise direction around the site \mathbf{r} of the dual lattice. We are still free to choose \tilde{V} to impose a global phase twist Δ_{μ} in the direction μ around the torus. The lowest energy $E_0(\Delta_{\mu})$ is 2π periodic in Δ_{μ} with a minimum at some Δ_{μ}^0 which depends on the particular sample. To introduce a spin domain wall perpendicular to x , one simply changes the twists from their best twist (BT) values $\Delta_{\mu}^0 \rightarrow \Delta_{\mu}^0 + \pi \delta_{\mu, x}$ and finds the minimum energy subject to these BC, which yields the energy with a spin defect $E_{SD}(L) > E_0(L)$. The spin defect energy $\Delta E_s^{\text{BT}}(L) \equiv E_{SD}(L) - E_0(L)$ is computed for different samples and sizes L and fitted to

$$\langle \Delta E_s^{\text{BT}}(L) \rangle \sim L^{\theta_s^{\text{BT}}} \quad (2)$$

to obtain the spin stiffness exponent θ_s^{BT} . A chiral domain wall is imposed by reflective BC [4,10] which means that there is a seam encircling the torus in (say) the y direction across which the spins interact as $\tilde{V} = V(\theta_i + \theta_j - A_{ij})$ which is equivalent to a reflection of the spins around some arbitrary axis. In principle, one can follow the same procedure as for the spin defect to obtain the chiral defect energy $\Delta E_c^{\text{BT}}(L) = E_{cD}(L) - E_0(L)$ where E_{cD} is the minimum energy with the modified interactions on a seam. However, there is no reason to expect that $E_{cD} > E_0$ as the BC defining E_0 may trap a chiral defect in some samples in which cases the modified interactions cancel the chiral defect and $E_{cD} < E_0$, as in fact does occur. We therefore define $\Delta E_c^{\text{BT}} = |E_{cD} - E_0|$, average this over disorder, and fit to $\langle \Delta E_c^{\text{BT}}(L) \rangle \sim$

$L^{\theta_c^{\text{BT}}}$ to obtain θ_c^{BT} . This does not affect ΔE_s^{BT} as both E_{SD} and E_0 contain identical chiral defects. The procedure described above using the phase representation of Eq. (1) is similar to that of most previous studies [2–4,6,8] except that these omit the minimization with respect to the twists Δ_{μ} , apply naive periodic and antiperiodic BC, and call the lowest energies E_p and E_{ap} . Neither of these BC is compatible with the GS and both must induce some excitation from E_0 . Nevertheless, the spin defect energy is defined as $\Delta E_s^{\text{RT}} \equiv |E_{ap} - E_p|$ and the spin stiffness exponent defined by $\langle \Delta E_s^{\text{RT}}(L) \rangle \sim L^{\theta_s^{\text{RT}}}$. We call this a random twist (RT) measurement as both BC are equivalent to some random choice of Δ_{μ} relative to Δ_{μ}^0 for each sample. There is no good reason to expect $\Delta E_s^{\text{RT}}(L)$ to scale as L^{θ_s} but if it does, there is less reason to expect any relation between θ_s^{RT} and θ_s^{BT} or θ_c .

The procedure in terms of the phase representation of the XY spin glass Hamiltonian of Eq. (1) is followed by previous studies. The aim is to obtain $\Delta E(L)$ by independently minimizing the Hamiltonian with respect to the θ_i to obtain E_D and E_0 . This requires finding essentially exact global minima for each sample to control the errors in $\langle \Delta E(L) \rangle$ to be purely statistical and $O(N^{-1/2})$ where N is the number of samples. If the minimization algorithm fails to find the true global minima, the errors in $\langle \Delta E(L) \rangle$ will be uncontrolled and very large, making the data point useless. Since the θ_i are continuous, one has to perform a numerical search of a huge configuration space, most of which does not even correspond to a *local* energy minimum. To reduce the volume of the space, we transform to a Coulomb gas (CG) representation which eliminates spin wave excitations and parametrizes the problem in terms of integer valued vortex or charge configurations, each of which is a local energy minimum. This reduces the space to be searched to a manageable size at the price of introducing long ranged Coulomb interactions between vortices. The potential $V(\phi)$ in Eq. (1) is taken as a piecewise parabolic potential equivalent to a Villain [21] potential at $T = 0$ with Hamiltonian $H = J \sum_{\langle ij \rangle} (\phi_{ij} - A_{ij})^2/2$ where $\phi_{ij} = \theta_i - \theta_j - 2\pi n_{ij}$ with $n_{ij} = -n_{ji}$ any integer on the bond ij . By a duality transformation [10,22,23], the CG Hamiltonian with periodic BC in the phases becomes

$$H = 2\pi^2 J \sum_{\mathbf{r}, \mathbf{r}'} (q_{\mathbf{r}} - f_{\mathbf{r}}) G(\mathbf{r} - \mathbf{r}') (q_{\mathbf{r}'} - f_{\mathbf{r}'}) + J(\sigma_x^2 + \sigma_y^2)/2L^2, \quad (3)$$

where

$$\begin{aligned} \sigma_x &= -2\pi [L(q_{x1} - f_{x1}) + \sum_{\mathbf{r}} (q_{\mathbf{r}} - f_{\mathbf{r}}) y], \\ \sigma_y &= -2\pi [L(q_{y1} - f_{y1}) - \sum_{\mathbf{r}} (q_{\mathbf{r}} - f_{\mathbf{r}}) x], \quad (4) \\ G(\mathbf{r}) &= \frac{1}{L^2} \sum_{\mathbf{k} \neq 0} \frac{e^{i\mathbf{k} \cdot \mathbf{r}} - 1}{4 - 2\cos k_x - 2\cos k_y}. \end{aligned}$$

Here, $\mathbf{r} = (x, y)$ denotes the sites of the dual lattice and $G(\mathbf{r})$ is the lattice Green's function. In Eq. (4), $k_\alpha = 2\pi n_\alpha/L$ with $n_\alpha = (0, 1, \dots, L-1)$. The topological charge, $q_{\mathbf{r}}$, is the circulation of the phase about the plaquette at \mathbf{r} and can be any integer subject to the neutrality condition $\sum_{\mathbf{r}} q_{\mathbf{r}} = 0$. The global frustration in the x direction $f_{x1} = \sum_{\square x} A_{ij}/2\pi$ is the circulation around the whole torus on the x bonds of plaquettes at $y = 1$ and q_{x1} is the global circulation of the phase. f_{y1} and q_{y1} are defined similarly. Periodic BC in the phases θ_i restrict q_{x1}, q_{y1} to be integers. A chiral domain wall is introduced by reflective BC [10] so that there is a seam encircling the torus in (say) the y direction across which the phases interact as $\tilde{V} = V(\theta_i + \theta_j - A_{ij})$, which is equivalent to a reflection of the original spins about some arbitrary axis. A more convenient form of the Hamiltonian for simulation purposes is by doubling the lattice in the x direction to a $2L \times L$ lattice with two chiral defects so that the extra half is a charge conjugated image of the original with Hamiltonian [10],

$$H_R = \pi^2 J \sum_{\mathbf{r}, \mathbf{r}'} (q_{\mathbf{r}} - f_{\mathbf{r}}) \tilde{G}(\mathbf{r} - \mathbf{r}') (q_{\mathbf{r}'} - f_{\mathbf{r}'}), \quad (5)$$

where $\tilde{G}(\mathbf{r})$ is the Green's function for a $2L \times L$ lattice with *periodic* BC and $q_{\mathbf{r}+L\hat{x}} = -q_{\mathbf{r}}, f_{\mathbf{r}+L\hat{x}} = -f_{\mathbf{r}}$.

To estimate the spin stiffness exponent θ_s , simulations were performed on a $L \times L$ lattice with Eq. (3) in two different ways. The first is a RT measurement by imposing standard periodic and antiperiodic BC corresponding to $\Delta_x = 0, \pi$, then fitting to $\langle \Delta E_s^{\text{RT}}(L) \rangle \sim L^{\theta_s^{\text{RT}}}$. This is just the procedure followed by all previous studies and, not surprisingly, gives essentially the same result $\theta_s^{\text{RT}} = -0.76 \pm 0.015$ [2–6,8] with sizes $L = 4, 5, 6, 7, 8$, and 10 and averaging over 2560 samples for $L \leq 8$ and 1152 for $L = 10$ (see Fig. 1). This does not exploit all the freedom implied by Eq. (3). One finds a global energy minimum by optimizing the BC by allowing the combinations $(q_{x1} - f_{x1})$ and $(q_{y1} - f_{y1})$ to vary independently over any integer or half integer. This corresponds to allowing the circulations of the phase difference and of A_{ij} around the two independent loops encircling the torus to vary. The absolute minimum energy E_0 is the GS energy (of a particular sample) which is realized by $f_{1x} = f_{1x}^0 = \Delta_x^0/2\pi$. A spin domain wall is induced by $f_{x1}^0 \rightarrow f_{x1}^0 + 1/2$. The energy minimum E_{sD} with these BC includes the spin defect energy. Fitting the difference, $\Delta E_s^{\text{BT}}(L) \geq 0$, to Eq. (2) yields $\theta_s^{\text{BT}} = -0.37 \pm 0.015$, averaging over the same number of samples as in the RT measurement. This is equivalent to making a gauge transformation to all bonds in the direction $\mu = (x, y)$ by $A_{ij} \rightarrow A_{ij} + \Delta_\mu/L$. The RT measurement keeps f_{x1} fixed or $\Delta_\mu = 0$, calling the lowest energy E_p , then changing $f_{x1} \rightarrow f_{x1} + 1/2$ and calling the resulting lowest energy E_{ap} and assuming the energy difference scales as $L^{\theta_s^{\text{RT}}}$. This procedure is equivalent to choosing an arbitrary gauge $A_\mu(\mathbf{r})$ to compute E_p and then E_{ap} is computed in the gauge $A_\mu + \pi \delta_{\mu,x}/L$.

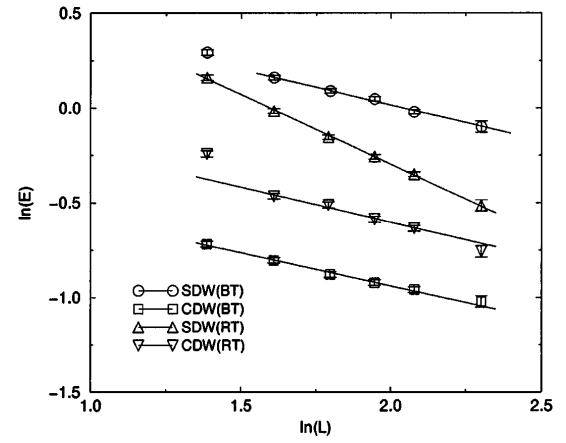


FIG. 1. Top to bottom: L dependence of ΔE_s^{BT} , ΔE_s^{RT} , ΔE_c^{RT} , and ΔE_c^{BT} , respectively, for $L = 4, 5, 6, 7, 8$, and 10. Solid lines are power-law fits.

The original problem of Eq. (1) is invariant under discrete gauge transformations modulo 2π so the RT measurement is performed in a *random* gauge while the BT measurement is done in the sample dependent gauge which minimizes the energy. We use simulated annealing [24,25] to estimate the energy minima, which is much more efficient than simple quenching to $T = 0$.

The chiral domain wall energy is also measured in two ways. Defining $\langle \Delta E_c^{\text{RT}} \rangle \equiv \langle |E_m - \langle E_m \rangle| \rangle$ [3] where $E_m = \min(E_p, E_{ap}) - E_R$ with E_R the GS energy with reflective BC gives the RT measurement for ΔE_c^{RT} and we obtain $\theta_c^{\text{RT}} = -0.37 \pm 0.015$. The other way is the BT measurement which is analogous to that for θ_s^{BT} when the absolute minimum energy is when the boundary terms in Eq. (3) vanish. Since the lowest energy of Eq. (5) may contain a chiral but not a spin domain wall, the BT condition will hold and any boundary terms must vanish. Even if, in general, there were boundary contributions to Eq. (5), they would vanish in the BT condition. Thus, a BT measurement of ΔE_c^{BT} is obtained from $|E_R^{\text{BT}} - E_0^{\text{BT}}|$ where E_R^{BT} is the minimum of Eq. (5) and E_0^{BT} is the minimum of Eq. (3). Fitting to $\langle \Delta E_c^{\text{BT}}(L) \rangle \sim L^{\theta_c^{\text{BT}}}$ yields $\theta_c^{\text{BT}} = -0.37 \pm 0.010$. This implies that $\theta_c^{\text{BT}} = \theta_s^{\text{BT}} \approx -0.37$ to within numerical accuracy, agreeing with the conjecture of Ney-Nifle and Hilhorst [10]. Note that the value of $\theta_s^{\text{RT}} \approx -0.76$ does not satisfy the conjecture. The only difference between the RT and BT measurements is in E_0 from Eq. (3) where E_0^{RT} is obtained with fixed random BC and E_0^{BT} by also minimizing with respect to the BC. E_{cD}^{BT} and E_{cD}^{RT} are both obtained from Eq. (5) and are identical because this is automatically a BT measurement for the special case of the spin glass as the boundary contributions to the energy vanish. Note that both measurements give identical values for the chiral exponent θ_c to within numerical uncertainty while the spin stiffness exponents θ_s^{BT} and θ_s^{RT} differ by a factor of 2. All 2D results are in Fig. 1.

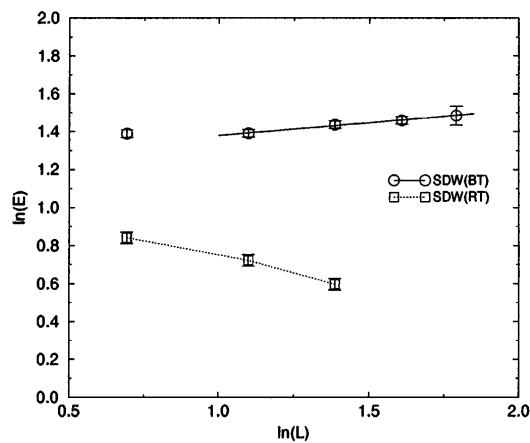


FIG. 2. ΔE_s^{BT} and ΔE_s^{RT} in 3D. The error in the $L = 6$ point is due to rather few samples. The solid line is a power-law fit and the dotted line is a guide to the eye.

Since the numerical estimates of θ_s^{BT} and θ_c^{BT} agree with the crucial test in 2D [10], we can regard this as supporting our contention that we have a good definition of the defect energies and our numerical method is fairly accurate. We have done simulations on the 3D XY spin glass to estimate the spin stiffness exponent θ_s and find $\theta_s^{\text{BT}} = +0.10 \pm 0.03$ with $L = 2, 3, 4, 5$, and 6 (Fig. 2). This is larger and more accurate than the estimate of Ref. [6]. The large error is due to fitting over only four data points. The negative slope of $\langle \Delta E_s^{\text{RT}}(L) \rangle$ for $L = 2, 3$, and 4 is expected to become positive at larger L [6]. At present, we have been unable to derive the 3D analog of Eq. (5), so we have no estimate of θ_c [6] in 3D.

Although we are unable to *prove* assertions such as the scaling ansatz, we believe that our BT method gives reliable estimates of the fundamental quantities $\theta_{s,c}$ in 2D and 3D. Our definition of the GS of a finite system does ensure that the fundamental disordering excitations have positive energy unlike the RT method. Also, the BT estimates agree with the analytic conjecture and the scaling ansatz $\langle \Delta E^{\text{BT}}(L) \rangle \sim L^\theta$ is obeyed very well in 3D unlike $\langle \Delta E^{\text{RT}}(L) \rangle$. They give a coherent, self-consistent picture which does not contradict any known result. One may object to our claims on the grounds that they are very BC dependent and that only the large L behavior is relevant. Since any simulation is limited to small L , a more relevant question is whether our BT scheme can constitute a smooth monotonic approach to this limit. This is beyond our expertise but we see no reason to believe the contrary and numerically $\langle E_{0,D}^{\text{BT}}(L) \rangle$ behave monotonically and smoothly with L .

The issue addressed here is the possible existence of a distinct thermodynamic phase at sufficiently low T by

appealing to the exponents $\theta_{s,c}$. In 2D an ordered phase is possible only at $T = 0$ but its *nature* is beyond the scope of this Letter. Earlier work [8] claims that in 2D the ordered phase has no long range order due to many degenerate ground states which leads to $\eta > 0$. This is inconsistent with the droplet picture [20] which has been verified analytically for a toy model [11] but not for more realistic models, which is a problem for the future.

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