Journal of Statistical Physics, Vol. 71, Nos. 1/2, 1993

Partition Function Zeros and the Three-Dimensional Ising Spin Glass

Gyan Bhanot[1,2] **and Jan Lacki**[1]

Received April 28, 1991; final October 21, 1992

We have computed the exact partition function of the 3D Ising spin glass on lattices of effective size $3\times3\times L_z$, $4\times4\times L_z$, and $5\times5\times L_z$ for L_z up to 9, and several random bond configurations. Studying the distribution of zeros of the associated partition functions, we find further evidence that these systems have a singularity in the thermodynamic limit.

KEY WORDS: Phase transitions; Ising spin glass; exact partition functions; helical boundary conditions.

Spin glasses are systems of magnetic impurities embedded in a background medium (see ref. 1 for a current review). The impurities move about slowly in the medium, and as they drift, the magnetic interaction between them randomly changes sign. The time over which the sign of the interaction changes is much longer than the time for a flip of the spin due to thermal effects. Further, the interaction strength falls off rapidly with distance. Hence, the simplest model for these systems is an Ising spin model with local interactions and random, quenched bond strengths $J_{ij}=\pm1$.

The free energy of such a system is given by

$$F(\beta)=\sum_J \log[Z(J,\beta)]\Big/\sum_J \tag{1}$$

where

$$Z(J,\beta)=\sum_\sigma \exp\left[-\beta\sum_{i,\mu}(1-\sigma_i J_{i,\mu}\sigma_{i+\mu})\right] \tag{2}$$

[1] School of Natural Sciences, Institute for Advanced Study, Princeton, New Jersey J 08540.
[2] Thinking Machines Corporation, Cambridge, Massachusetts 02142.

0022-4715/93/0400-0259$07.00/0

where σ_i is an Ising spin at site i, μ denotes direction, and J denotes a sum over random bond configurations.

The sum over spin configurations in Eq. (2) can be transformed into one over the total energy by changing variables to

$$E = \tfrac{1}{2} \sum_{i,\mu} (1 - \sigma_i J_{i,\mu} \sigma_{i+\mu}) \tag{3}$$

The Jacobian of this change of variables is a function $P(E)$, which is the number of states of the system with energy E. Thus,

$$Z(J, \beta) = Z(J, u) = \sum_{E=0}^{N_l} P(E)\, u^E \tag{4}$$

where N_l is the number of bonds and $u = e^{-2\beta}$. We will compute the coefficients $P(E)$ exactly. Among other things, we are then able to study the analytic properties of F by looking at the zeros of (4). The method we use is one originally suggested by Binder[2] and improved by Bhanot[3] and Creutz.[4] It uses a transfer matrix technique to build up the partition function layer by layer by stacking transverse 2D slices of L_{xy} spins along a third longitudinal direction. The utility of the method is that it allows the calculation to be done on lattices which would be impractical to study by a direct enumeration of spin states.

In the method of ref. 3 the computer memory required is proportional to $2^{L_{xy}} E_{\max}$, where $E_{\max}$ is the energy of the most energetic spin configuration. In order to minimize L_{xy}, we use a method invented by Creutz,[4] which allows a system with a few spins to mimic a much larger 2D system, in a sense that will become clear later. The method of Creutz is based on using a special type of helical boundary condition. Let us consider an example. As shown in Fig. 1, consider 13 spins along a one-dimensional

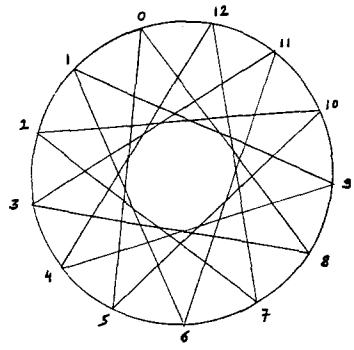


Fig. 1. The 13-spin helix with its x, y bonds.

chain. Let us label the spins from 0 to 12. Nearest neighbors in the x direction have a label differing by unity (modulo 13). The trick of Creutz is to define nearest neighbors in the y direction to have an index differing by 5. Thus, the neighbors of spins 0, 1, 2,... in the y direction are the spins 5, 6, 7,.... Note that by doing this we have ensured that the shortest closed path is of length 5. This means that when computing the low-temperature expansion, finite-size effects appear at the same order on our 13-site lattice as on 5×5 lattice with periodic boundary conditions. It is in this sense that we say that the 13-site system 'mimics' a 5×5 periodic lattice. In general, let n be the smallest path on the L_{xy} lattice that is closed due to finite lattice size. Then, the L_{xy} lattice 'mimics' an $n \times n$ periodic lattice in the sense that they have the same low-temperature behavior upto finite-size corrections.

Following Creutz, we call the lattice in Fig. 1 a 13/5 lattice. Similarly, one can show that 8/3, 18/5, 25/7, 32/7, and 42/16 lattices are equivalent to 4×4, 6×6, 7×7, 8×8, and 9×9 periodic lattices, respectively. In this paper, we consider 3 D Ising-like spin glasses where the x, y transverse slice consists of one of the 5/3, 8/3, or 13/5 helixes, stacked up respectively 7, 8, and 9 times along the z direction.

Following refs. 3 and 4, we build up the partition function by first enumerating all the states of the bottom transverse slice and then adding spins one by one, layer by layer. We put cold layers ($\sigma_i = 1$) at the ends in the z direction and compute $P(E)$ by explicitly keeping track of how many states have a given energy as the partition function is built up. In the case of the Ising model (all the bonds are $+1$), the cold boundary conditions force all the spin configurations to have even energies, i.e., (4) is an even polynomial. Such is not the case for an arbitrary bond configuration, but, as we will shortly see, another closely related and intriguing effect takes place.

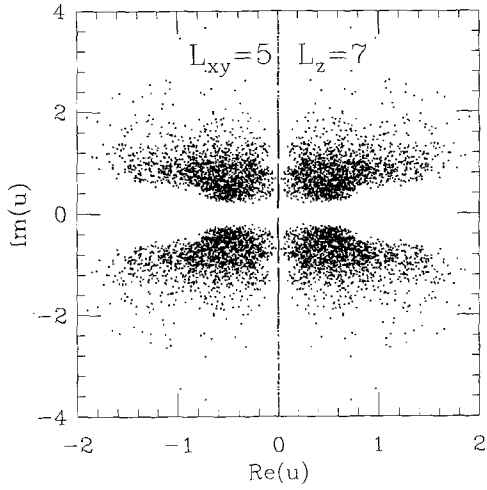
One can easily parallelize the construction of the partition function by vectorizing over the $2^{L_{xy}}$ states of L_{xy} transverse spins. We used an $8K$ Connection Machine CM-2 with 1 Gbyte of memory for our calculations. Our program took about 10 min per bond configuration to find $P(E)$ for z up to 9 in the case of $L_{xy} = 13$. We generated Z for 200, 100, and 30 random bond configurations for $L_{xy} = 5, 8, 13$.

As defined in Eq. (4), the partition function is a finite polynomial in u and is therefore completely determined by its zeros. Note also that the free energy in Eq. (1) can be written as the log of the product of partition functions over bond configurations. Thus,

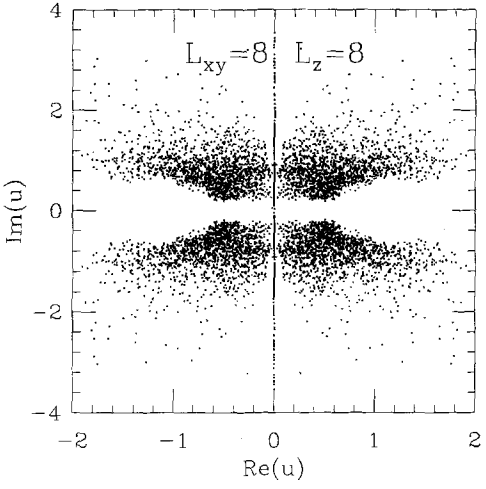
$$F \sim \log \left[\prod_J Z(J, u) \right] \tag{5}$$

Hence, the analytic structure of F may be displayed by plotting the zeros of Z for all bond configurations together in the complex u plane.

In Fig. 2 we show our results for the zeros of our various systems for the largest number of layers in the z direction. The zeros were computed using very high-precision arithmetic in Mathematica and were checked by ensuring that they solve $Z(J, u_i) = 0$. For each configuration all the zeros

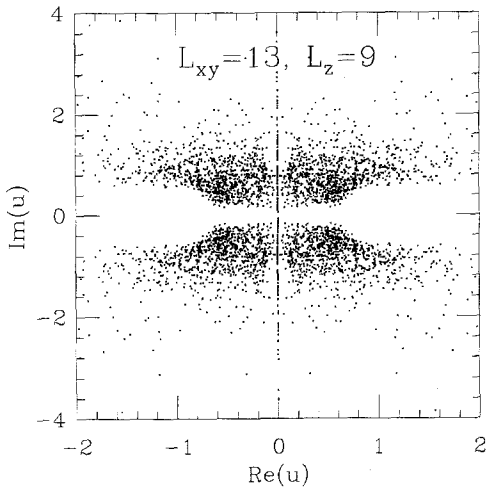


(a)



(b)

Fig. 2. All the zeros for (a) ($L_{xy} = 5$, $L_z = 7$), (b) ($L_{xy} = 8$, $L_z = 8$), and (c) ($L_{xy} = 13$, $L_z = 9$).



(c)

Fig. 2. (*Continued*)

were computed and this allowed us to observe some curious properties of these zeros.

We found that for each random configuration there are always N_z^- zeros at $u=-1$ with N_z^- equal to the total number of z directed bonds that are set to -1. Apart from these, the remaining zeros are symmetric with respect to reflection both in the real *and* the imaginary u axes. Reflection symmetry in the real axis is trivial because the $P(E)$'s are real. However, reflection symmetry in the imaginary axis is nontrivial. This property implies that the partition function $Z(J, u)$ factors into a term $(1+u)^{N_z^-}$ times a polynomial with only even powers of u. This fact was checked for all the bond configurations by explicit algebraic factorization (using Mathematica) of the partition functions. This curious property is quite evident in Fig. 2, where we plot all zeros except the ones at $u=-1$ for all bond configurations. We do not have any clear explanation for this factorization. We note that there is nothing special about the negative bonds themselves: The fact that there are N_z^- zeros at $u=-1$ is related to the fact that we chose the boundary condition $\sigma_i=1$ on both ends. Indeed, if we set $\sigma_i=1$ on the bottom layer and $\sigma_i=-1$ on the top, $Z(J, u)$ has a factor

$$(1+u)^{N_z^+}$$

where N_z^+ is the number of $+1$ bonds in the z direction. What is intriguing is the fact that there is precisely one factor $(1+u)$ per vertical bond (of the

sign determined by the given choice of boundaries). The meaning of the remaining even polynomial is obscure.

As Fig. 2 indicates, the zeros for Re(u) form a shelf with a finite Im(u). A nonanalyticity of the free energy would result if the shelf of zeros descended to the real-u positive half-axis in the thermodynamic limit. In our numerical experiment, we have two parameters controlling the size of the system. For a finite, fixed transverse size L_{xy}, we can increase the longitudinal size L_z. One would then expect the shelf to move closer to the real u axis but eventually to level off, as there cannot be a singularity in one-dimension. This is indeed what is observed, as is shown in Fig. 3. This figure has been obtained computing the Im(u) of the zero closest to the real axis for each bond configuration, then averaging over the configurations and plotting against L_z.

Let us define the characteristic linear dimension $L = (L_{xy} L_z)^{1/3}$ for a lattice of size $L_{xy} \times L_z$. For L_{xy} and L_z both large, as one approaches the thermodynamic limit, the distance from the closest zero to the positive u axis should scale as $A + BL^{-1/\nu}$, where ν is the correlation length and A and B are u-dependent functions[5] with A purely real. The averages (over bond configurations) of Im(u) for the zero closest to the positive u axis plotted against L^{-1} are shown in Fig. 4. The results strongly suggest a phase transition in the thermodynamic limit because the average of Im(u) seems to vanish in this limit. To determine ν, we make a fit of the data in Fig. 4 to $aL^{-1/\nu}$ keeping only those points which have the underlying L_z

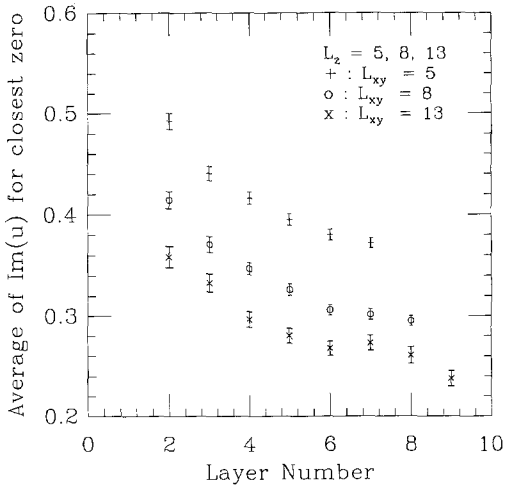


Fig. 3. The average (over configurations) of the imaginary part of the closest zero as a function of L_z.

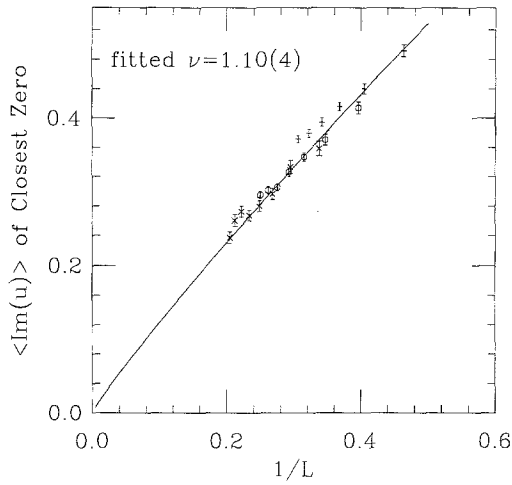


Fig. 4. The average of the imaginary part of the closest zero as a function of L^{-1}. The solid line is a fit to $aL^{-1/\nu}$.

less than $n+1$, where n is the length of the shortest closed path in the xy plane (as determined by L_{xy}). This is to avoid making the lattice look one dimensional (see Fig. 3). The solid line in Fig. 4 shows the fit. The fitted value is $\nu = 1.10(4)$, to be compared with $\nu = 1.4$ obtained from Monte Carlo simulations.[6] The discrepancy is probably a systematic error due to the relatively small L values we used. An estimate of the critical temperature can be obtained by plotting the average of the real part of the

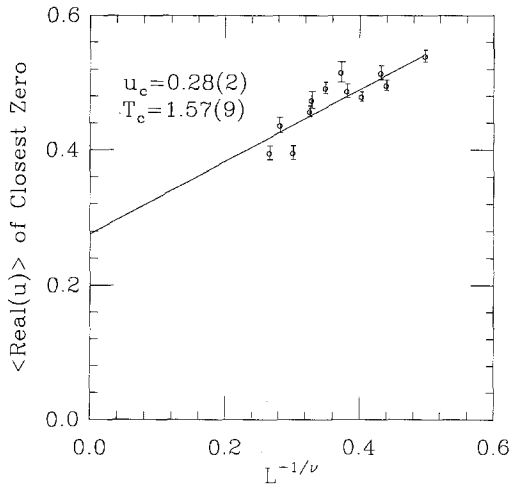


Fig. 5. Fit of the average real part of the closest zero to $c + dL^{-1/\nu}$.

closest zero against $L^{-1/\nu}$ and making a linear fit. This is shown in Fig. 5 with the resulting intercept $u_c = 0.28(2)$, implying $T_c = 1.57(9)$.

From our partition functions, one can also study the properties of the ground state, in particular the ground-state energy and the ground-state degeneracy. Figure 6 shows the average energy E_0 of the ground state as a function of the volume $V = L_{xy}L_z$. A fit to $E_0 = a + bV$ has an excellent χ^2 and the slope gives $E_0/V = 0.742(2)$.

In Fig. 7 we show the average degeneracy d of the ground state as a function of the volume. We made fits to $d = AV^{\rho}$ and $d = Be^{cV}$. Both fits have a good χ^2 and are shown in Fig. 7. The fitted parameter values are $(A = 0.07(1), \rho = 1.51(5))$ and $(B = 2.3(1), c = 0.047(1))$. The issue of which form is correct is important (e.g., for spin-glass models of neural networks) and can be resolved by studying larger systems.

As mentioned earlier, the memory required to compute Z scales like $2^{L_{xy}}$, which saturates most computers for rather small L_{xy}. However, we have found a way to construct even larger effective lattices by pushing the helix method one step further. Consider a set of points along a helix and define nearest neighbors along the x, y, z directions to be h_x, h_y, h_z steps away from each point. It is easy to show that one can make the shortest closed path rather with modest values for h_x, h_y, h_z. Indeed, $h_x = 7$, $h_y = 11$, $h_z = 12$ mimics a $7 \times 7 \times 7$ periodic system. Since the storage required to study this system by our method goes like 2^{h_z}, one can be optimistic that one can study rather large systems in this way. An interest-

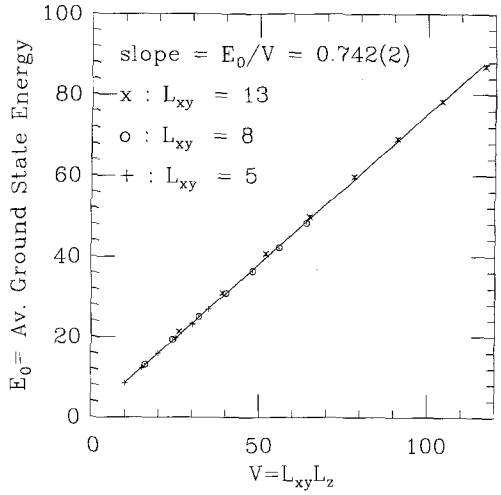


Fig. 6. The average energy of the ground state as function of the volume $L_{xy}L_z$. The curve is a least squares fit to a straight line.

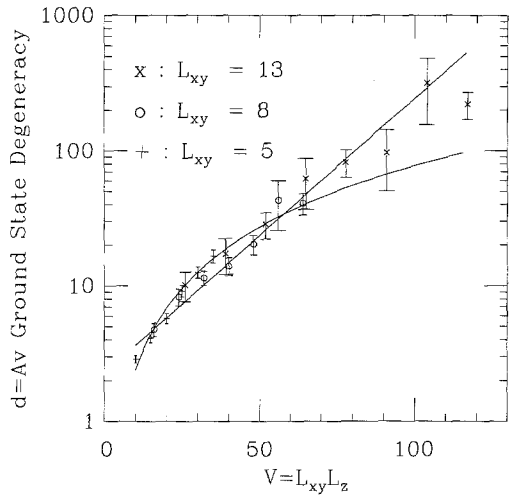


Fig. 7. The degeneracy of the ground states as a function of the volume $L_{xy}L_z$. The straight line is a fit to $d \sim e^{cV}$, the curve is a fit to $d \sim V^p$.

ing application of these helical lattices is to construct large orders of low-temperature expansions for the three-dimensional Ising model. Using this method, in collaboration with M. Creutz, we have computed the low-temperature series for the average energy per bond of the 3D Ising model to 50 excited bonds.[7]

ACKNOWLEDGMENTS

The work of G.B. was partly supported by U.S. DOE grant DE-FG02-90ER40542; the research of J.L. is partly supported by the Swiss National Scientific Fund. We thank Thinking Machines Corporation for generous amounts of time on their computers.

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