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Exact integer algorithm for the two-dimensional $\pm J$ Ising spin glass

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We describe an exact integer algorithm to compute the partition function of a two-dimensional $\pm J$ Ising spin glass. Given a set of quenched random bonds, the algorithm returns the density of states as a function of energy. The computation time is polynomial in the lattice size. We investigate defects, low-lying excitations, and zeros of the partition function in the complex plane. We also discuss the potential to examine other types of quenched randomness.

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The last 15 years have witnessed a great deal of work on spin glasses [1,2]. Nevertheless, the description of the phase transition and the nature of the ordered state remain controversial [3–6]. The starting point for most theoretical work is the Edwards-Anderson Hamiltonian [7]

$$\mathcal{H}[\{\sigma_i\}] = \sum_{i,j} J_{ij}\sigma_i\sigma_j \quad , \tag{1}$$

where the J_{ij} are quenched random variables and the σ_i are Ising spins on a regular lattice. Interactions with infinite range [8] lead to a solution with broken replica symmetry [2]. It is not known, however, to what extent this mean-field result captures the behavior of short-range interactions [4,9].

A widely studied model is the $\pm J$ spin glass [10], in which the sign of each bond is random but its magnitude fixed. In two dimensions, the $\pm J$ spin glass with nearest-neighbor interactions exhibits a phase transition only at zero temperature [11]. The properties of this $T = 0$ transition have been studied by high-temperature expansions [12], Monte Carlo (MC) simulations [13–15], and exact calculations of partition functions on small lattices [11,16]. In this paper, we describe an exact integer algorithm to calculate the partition function of this system. The algorithm takes as input a set of quenched random bonds and returns the density of states as a function of energy. In contrast to other exact methods [11], the computation time of our algorithm is polynomial in the lattice size [17]. Partial output for a 10×10 $\pm J$ spin glass is shown in Table I. Here we discuss only the basic elements of the algorithm; further details will be reported elsewhere [18]. We also refer the interested reader to other integer algorithms [19–21], based on transfer-matrix methods on finite lattices that compute exact partition functions of Ising systems.

We consider Ising spins $\sigma_i = \pm 1$ on an $L \times L$ lattice. The Hamiltonian is given by Eq. (1), with the sum restricted to pairs of nearest neighbor spins. The quenched random bonds J_{ij} are chosen from the bimodal distribution

$$\mathcal{P}(J_{ij}) = \frac{1}{2}\delta(J_{ij} - J) + \frac{1}{2}\delta(J_{ij} + J), \tag{2}$$

with $J > 0$. On a lattice with periodic boundary conditions (BC's), there are exactly $2N$ bonds and $N = L^2$ spins. The partition function is given by

$$Z = \sum_{\{\sigma_i\}} e^{-\beta\mathcal{H}[\{\sigma_i\}]} \tag{3}$$

with $\beta \equiv 1/T$. A high-temperature expansion of the partition function yields a power series in $\tanh(\beta J)$ whose terms have a diagrammatic representation as closed graphs on the square lattice [22]. Motivated by this diagrammatic representation, Kac and Ward [23] transformed the problem of summing the high-temperature series into one of evaluating a local random walk. In particular, they showed how to use a $4N \times 4N$ *hopping matrix* to compute the coefficients of the high-temperature expansion [22]. The columns of this hopping matrix correspond to directed bonds on the square lattice. The final result of Kac and Ward, valid in the thermodynamic limit, is that

$$\frac{\ln Z}{N} = \ln[2\cosh^2(\beta J)] - \frac{1}{2N}\sum_{\ell=0}^{\infty}\frac{1}{\ell}\mathrm{tr}(U^\ell)\tanh^\ell(\beta J), \tag{4}$$

where $\mathrm{tr}(U^\ell)$ denotes the trace of the ℓth power of the hopping matrix. These traces count closed loops of length ℓ on the square lattice, reproducing the high-temperature expansion of Z. Equation (4) can be written in the more compact form

$$Z = 2^N \cosh^{2N}(\beta J)\sqrt{\det[1 - U\tanh(\beta J)]} \tag{5}$$

TABLE I. Partition function, $Z = \sum_E g(E)e^{-\beta E}$, for a 10×10 $\pm J$ spin glass. The calculation took 110 s on an INDIGO 4000 workstation.

E/J	$g(E) = g(-E)$
142	1714
138	393704
134	26810830
⋮	⋮
10	1113882635377304453900417184 18
6	13061878960842792764584692738 2
2	14144047506466710966045617415 8

using standard matrix identities. The problem is thus reduced to evaluating the determinant of a $4N \times 4N$ matrix.

For models with translational symmetry, one can use Fourier transforms to diagonalize this matrix and obtain analytic results in the thermodynamic limit. Of course, the same techniques do not apply to random systems, such as the $\pm J$ spin glass. We can, however, use the Kac-Ward method to compute the partition function for a $\pm J$ spin glass of *finite size*. In this case, Eq. (5) must be slightly modified to incorporate periodic BC's. The correct result, based on the combinatorics of closed loops on periodic lattices [24], is $Z = (-Z_1 + Z_2 + Z_3 + Z_4)/2$, with

$$Z_\alpha = 2^N \cosh^{2N}(\beta J) \sqrt{\det[1 - U_\alpha \tanh(\beta J)]}. \qquad (6)$$

Here, U_α are four distinct $4N \times 4N$ hopping matrices related to one another by boundary transformations.

We have implemented this algorithm on the computer as follows. Given a set of bonds $\{J_{ij}\}$, we first construct the $4N \times 4N$ matrices U_α and compute the traces $\mathrm{tr}(U_\alpha^\ell)$ for $\ell \leq N$. This step of the algorithm is the most computationally intensive. The coefficients of the series expansions for $\ln Z_\alpha$ are related to the traces by Eq. (4). Next, we compute the high-temperature series for Z. This is done by exponentiating the series for $\ln Z_\alpha$ and taking the linear combination that incorporates periodic BC's. The high-temperature expansion for Z is a polynomial in $\tanh(\beta J)$ with integer coefficients; the last term, of order $2N$, is derived from the graph that traverses every bond on the square lattice. These $2N$ coefficients have an end-to-end symmetry that enables one to compute them from the first N powers of the hopping matrix. Finally, we expand powers of $\cosh(\beta J)$ and $\tanh(\beta J)$ and rewrite Z as a polynomial in $e^{-\beta J}$; the end result $Z = \sum_E g(E) e^{-\beta E}$ yields the density of states. For an Ising model with $\pm J$ bonds, we can perform all these operations using only integer arithmetic.

The algorithm has several desirable features. Like the numerical transfer-matrix (TM) method [11], it returns an exact result and avoids the sampling errors of MC simulation. Another bonus is that it executes in polynomial time [17]. Computing the traces requires $O(N^3)$ arithmetic operations on integers of order 2^N, so that the computation time scales as $\tau \sim N^\delta$, with $3 < \delta < 4$. [Indeed, the computation of the traces can be broken down into $O(N)$ independent processes, so that a faster, parallel implementation of the algorithm on a supercomputer or spread across several workstations should be possible.] This stands in contrast to the TM method [11], which must keep track of 2^L spin configurations to compute the partition function on a strip of width L. We look at larger square lattices than previous TM studies [11,16]. With the integer density of states, we can also compute new quantities, such as the roots of the partition function in the complex plane [21].

We examined lattices of size $L = 4$ to $L = 36$. Several realizations of randomness were studied: 8000 for $L = 4, 6, 8$; 2000 for $L = 10, 12, 14$; 800 for $L = 16, 18$; 80 for $L = 20, 22, 24$; and 4 for $L = 32, 36$. We performed quenched averages by assigning an equal probability to each random sample: $\overline{\theta} = (1/S) \sum_s \theta_s$. To reduce the amount of statistical error, we only considered lattices in which exactly half the plaquettes were frustrated [11]. For the average ground state energy and entropy per spin, we find $\overline{e_0}/J = -1.404 \pm 0.002$ and $\overline{s_0} = 0.075 \pm 0.002$. These results are consistent with previous MC [13,14] and TM [16] estimates.

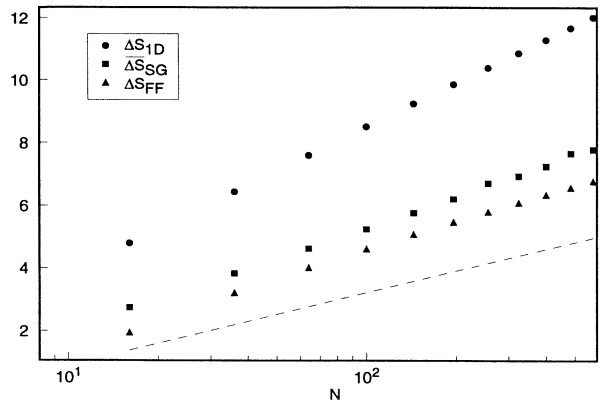

FIG. 1. Scale dependence of the entropy difference between the ground state and the lowest excited states for the 1D Ising model, the 2D FF model, and the 2D $\pm J$ spin glass. The dashed line shows $\ln(N/4)$.

We also used the algorithm to study the number of low-level excitations. On a lattice with periodic BC's, the lowest excited state has an energy $4J$ above the ground state. The quantity $e^{\Delta S} = g(E_0 + 4J)/g(E_0)$ measures the degeneracy ratio of excited and ground states. Figure 1 shows a semilog plot of $\overline{\Delta S}_{\mathrm{SG}}$ versus the number of spins N. The fact that $\overline{\Delta S}_{\mathrm{SG}}$ grows faster than $\ln N$ suggests that the low-lying excitations of the $\pm J$ spin glass involve spin flips on large length scales.

The abundance of low-lying excitations affects the low-temperature behavior of the heat capacity. In a finite system with energy gap $4J$, the heat capacity vanishes as $C \sim \beta^2 e^{-4\beta J}$. As pointed out by Wang and Swendsen [13], this behavior can break down in the thermodynamic limit. The 1D Ising model with periodic BC's shows how this can happen: the energy gap is $4J$, but the heat capacity of an infinite system vanishes as $C_{\mathrm{1D}} \sim \beta^2 e^{-2\beta J}$. The anomalous exponent reflects the fact that the number of lowest excited states grows as N^2. From MC and TM studies, Wang and Swendsen [13] conclude that $C_{\mathrm{SG}} \sim \beta^2 e^{-2\beta J}$ for the 2D $\pm J$ spin glass as well. For purposes of comparison, we have included data for the 1D Ising model in Fig. 1. The disagreement in slope between ΔS_{1D} and $\overline{\Delta S}_{\mathrm{SG}}$ leads us to suggest a different form for C_{SG}. As motivation, we appeal to another exactly soluble model with a phase transition at $T = 0$: the fully frustrated (FF) Ising model on a square lattice [25]. On a periodic lattice, the lowest excited states of the FF model have energy $4J$ above the ground state. The large number of low-lying excitations, however, causes the heat capacity to vanish as $C_{\mathrm{FF}} \sim \beta^3 e^{-4\beta J}$. Note the extra power of temperature. Comparing ΔS_{FF} and $\overline{\Delta S}_{\mathrm{SG}}$ in

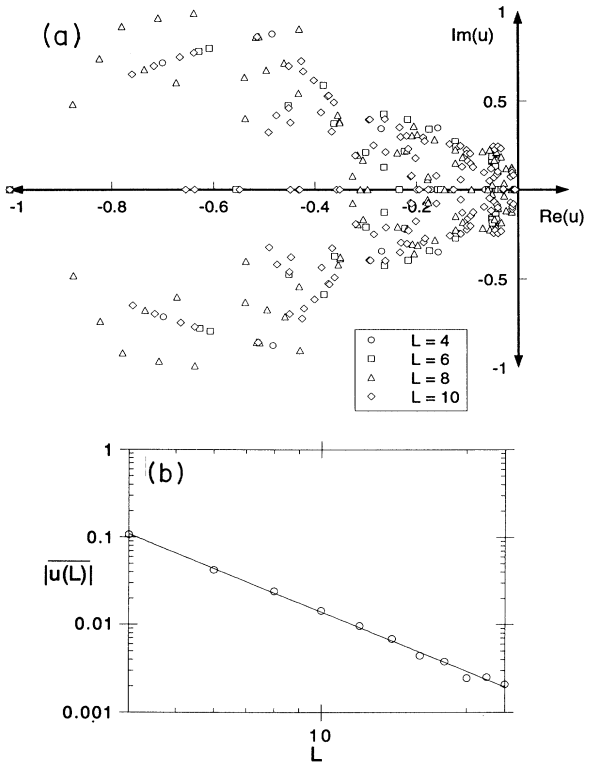

FIG. 2. (a) Roots of partition functions in the complex $u = e^{-4\beta J}$ plane. (b) Scale dependence of the smallest root.

Fig. 1, we suspect a similar behavior may describe the $\pm J$ spin glass, e.g., $C_{\rm SG} \sim \beta^{2+\rho} e^{-4\beta J}$ with $\rho \neq 0$. As we shall see below, there are other reasons to favor this form.

One way to investigate a phase transition is to look at the zeros of the partition function in the complex temperature plane [26]. The condensation of these zeros onto the real axis in the thermodynamic limit signals the existence of a phase transition. We found the zeros of Z for the $\pm J$ spin glass on four lattices of size $L = 4, 6, 8$, and 10. Figure 2(a) shows these zeros in the $u = e^{-4\beta J}$ complex plane; they condense around the origin, indicating a phase transition at $T = 0$. The zeros of partition functions are subject to finite-size scaling [27]. At a finite-temperature phase transition, the complex zero $u(L)$ closest to the positive real axis obeys $|u(L) - u_c| \sim L^{-y_t}$; likewise, the correlation length diverges as $\xi \sim (T - T_c)^{-\nu}$, with $\nu = 1/y_t$. On the other hand, at a $T = 0$ phase transition, such as in the 1D Ising model or 2D FF model, one finds $|u(L)| \sim L^{-y_u}$ with $\xi \sim u^{-1/y_u}$.

In the $\pm J$ spin glass, we observed that, for most realizations of randomness, the smallest root $u(L)$ fell on the negative real axis. Figure 2(b) shows a log-log plot of $\overline{|u(L)|}$ versus lattice size L, where the average was for computational reasons [28] restricted to realizations with $\mathrm{Im}[u(L)] = 0$. The fit shows $y_u = 2.2 \pm 0.1$; this suggests to us that the correlation length in the $\pm J$ spin glass diverges as $\xi \sim e^{2\beta J}$. Additional powers of temperature

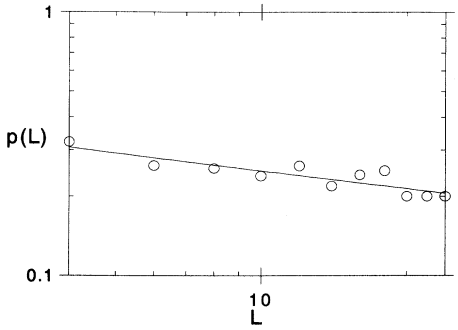

FIG. 3. Scale dependence of the fraction, $p(L)$, of effective block couplings with $J' \neq 0$.

and/or finite-size effects might explain the slight deviation from $y_u = 2$ in Fig. 2(b). Note that this behavior for the correlation length is consistent with hyperscaling and our claim that, up to powers of temperature, the heat capacity diverges as $C \sim e^{-4\beta J}$. It also suggests a lower critical dimensionality $d_l = 2$ for the $\pm J$ spin glass. Our result disagrees with previous studies [13,15,16] that report $\xi \sim T^{-\nu}$, with $\nu \approx 2.6$–2.8.

A great deal of information on spin glasses has been obtained by examining "defects" (droplets) in finite systems. The cost of a defect of size L is related to the difference in free energies with periodic and antiperiodic BC's. At $T = 0$, this reduces to the difference in energy between the ground states. On an $L \times L$ lattice, the defect energy measures the effective block coupling [3–6,9] J' on length scale L. Let $p(L)$ be the fraction of $L \times L$ blocks for which $J' \neq 0$. Scaling arguments [5] suggest that $p(L) \sim L^{-\eta}$, where η is the critical exponent that characterizes the power law decay of correlations $\overline{\langle \sigma_0 \sigma_L \rangle^2}$ at $T = 0$. Plotting $p(L)$ versus L (Fig. 3), we find $\eta = 0.22 \pm 0.06$ in agreement with previous results [5,13,15]. Besides the defect energy, we also looked at the defect entropy δS_L, i.e., the difference in zero-temperature entropies with periodic and antiperiodic BC's. The data in Fig. 4 show $\overline{\delta S_L^2} \sim L^{2y_S}$ with $y_S = 0.49 \pm 0.02$. This is curiously close to the result $\delta S_L \sim L^{1/2}$, expected if entropy changes due to reversing the different bonds along the boundary are statistically independent.

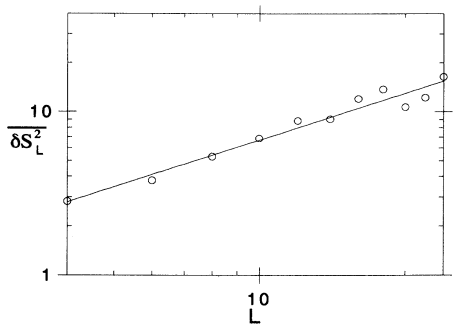

FIG. 4. Scale dependence of the mean square defect entropy.

In summary, we have developed an exact integer algorithm to compute the partition function of the 2D $\pm J$ spin glass in polynomial time. The algorithm complements the numerical TM method [11] and can serve as a strict check on MC techniques [13,14]. It can also be used to study a variety of other outstanding problems in the physics of 2D random systems. An obvious extension of this work is treating Ising models with $\pm J$ and/or missing bonds. A large number of random bond and percolation problems fall into this category. It would also be interesting to vary the concentration of frustrated plaquettes on the square lattice [11]. As a final note, we point out that a determinant, analogous to the one in Eq. (5), can be used to compute the partition function of any 2D planar Ising model in polynomial time [17]. The restriction to $\pm J$ bonds is only necessary to obtain an exact integer result [20,21]. For continuously distributed random bonds, one can use floating-point techniques to evaluate the determinant, and hence the partition function, at any given temperature. Hopping matrix formulas also exist for spin-spin correlations in 2D Ising models [29], making it possible to study magnetic susceptibilities. Polynomial-time algorithms based on these ideas should therefore complement well-established methods in the further study of 2D Ising models with quenched randomness.

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