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LETTER TO THE EDITOR

Multispin coding for spin glasses

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Abstract. We present a multispin coding algorithm for the 2D $\pm J$ spin glass model. It is a straightforward generalisation of Vichniac's Q2R Ising model. In contrast to that, however, it is not strictly deterministic and energy conserving, so that no problems with ergodicity arise. Numerical results are given for the ground state reached by simulated annealing. They are in good agreement with previous results.

Spin glasses [1] are a prime testing ground for optimisation methods in complex situations [2]. In particular, it is non-trivial to obtain the correct ground-state energy and entropy. Actually, it has been shown [3] that for 2D spin glasses this requires only polynomial time, i.e. it is not an NP problem. Nevertheless, the best available estimates seem to be from the transfer matrix method [4, 5] (the effort for which increases exponentially with size) and from simulated annealing. In the latter, one starts with a finite temperature, approaches thermal equilibrium at this temperature by Monte Carlo simulation, and then decreases temperature in small steps. As it was suggested [2] that simulated annealing might be very efficient also in other complex optimisation problems, it seems useful to understand it as well as possible in spin glasses.

The most precise results obtained up to the present in this way [6] have used the standard Metropolis algorithm. Recently, other methods for simulating spin systems have been developed which seem to be much more efficient when applied to the standard Ising model. These include the microcanonical models of Creutz [7, 8] and, as their ultimate simplification, the Q2R model of Vichniac [9].

In the Q2R model, the lattice is divided into two sublattices in a checkerboard fashion, and spins are updated alternatively on the two sublattices. The updating is such that spins are flipped if and only if the flip does not change the energy. Thus the evolution is purely deterministic, requiring no random number generators. The advantage therein is that the updating can be made simultaneously on many spins, by using only one bit of a computer word per spin, making the algorithm extremely fast [10, 11]. More precisely, only eight logical operations were necessary in [10] to update one computer word. The disadvantages are on the one hand that finite-size corrections seem larger due to the exact energy conservation. On the other hand, the model is not strictly ergodic. This does not seem to pose problems close to the critical point [11], but it should lead to severe problems at low temperatures.

In the present letter, we show that a simple modification of the Q2R model, preserving the advantages but avoiding the disadvantages, can be applied to the $\pm J$ spin glass at low temperature. This is defined by the energy

$$H = J \sum_{\langle i,k \rangle} \varepsilon_{ik} s_i s_k \qquad \varepsilon_{ik} = \pm 1 \qquad J = 1. \tag{1}$$

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On an infinitely large lattice, all horizontal bonds can be arranged by a gauge transformation to be ferromagnetic. The signs of the vertical bonds remain still completely random, and each bond can be represented by one bit. Assume the computer has N-bit words and the lattice has a width L which is a multiple of $2N$. Then, we need L/N words for each row of spins and L/N other words for the row of vertical bonds below. To take into account the random bonds, one needs just two additional Boolean operations per N spins for each update. (The gauge setting all horizontal bonds ferromagnetic could be avoided at the expense of one more word per N spins and two more Boolean operations.)

In order to improve the ergodicity, we do not flip spins each time when this would conserve energy, but only with probability $\frac{1}{2}$. This might seem to destroy the main advantage that simulation is faster when no random number generators are needed. But since we need only a single bit per spin set randomly to 0 or 1, this is also very fast. We need one random integer for each update of N spins and one more logical AND. The resulting increase of the updating time is less than 50%.

Up to this stage, we need 11 logical operations plus one random integer to update N spins.

The last modification was to break exact energy conservation, changing thus from the microcanonical to roughly the canonical ensemble. The drawbacks of the microcanonical ensemble as described above are as follows.

(a) Large finite-size corrections. This follows simply from the fact that a small system does not have the energy fluctuations it would have if it were part of a large system. In the canonical ensemble, a small system is in this way more similar to a part of an infinite one.

(b) Slow relaxation due to trapping in local minima. Jumps between local minima should be enhanced if the energy can fluctuate locally in space. In the above microcanonical model, the energy in any region of space can fluctuate only by being transferred through the boundary, which is slow compared to the fluctuations in a canonical model.

Since we are interested in the ground state and use non-zero temperatures only in auxiliary steps during the 'cooling down', we indeed do not need the exact canonical ensemble. A fast algorithm whose equilibrium state is a good approximation to the canonical ensemble is the following. When a spin flip decreases the energy, we perform it. If it leaves the energy constant, we perform it with probability $\frac{1}{2}$ as described above. Finally, if the flip would increase the energy, we do the flipping with a probability p independent of the energy increase. This probability is essentially the Boltzmann factor, $p \approx \exp(-2J\beta)$, for the smaller of the two increases. A fast way of performing these flips consists in storing an array of bit masks with bits set to '1' randomly with probability p, and making logical AND with these bit masks. In order to avoid any problems related to the finiteness of the array of bit masks, we scrambled them before each application. This needed two more random numbers and one SHIFT per updating of N spins.

The final algorithm needed three random numbers and 24 logical operations for each updating of N spins. On a Cyber 170/175, one updating required 0.82 μs per spin. The final relaxation to the ground state at $T = 0$ was somewhat simpler and took only 0.44 μs.

The cooling strategy was essentially the same as in [6], although different strategies have been discussed recently [12]. We started at temperature $T = 1.2$. In steps of $\Delta T = 0.14$, we went down to $T = 0.5$. Below this temperature, thermal effects were

estimated to be negligible within our statistics, and thus we continued with $T=0$. In one run, the number t of iterations at each of these seven temperatures was the same. Energies reached in this way depend evidently on the cooling rate $\Delta T/t$. Results for various rates are given in figure 1 and table 1. Each data point in figure 1 is obtained from a large number of independent runs on a lattice of 240×240 spins. The number of runs for each t is also given in table 1. Also plotted in figure 1 are the values of [6].

In [6] it was claimed that the energies (per spin) reached in such a cooling procedure behave as

$$E(t)=E_0+\text{constant}\times t^{-x} \tag{2}$$

with $x\approx0.2$–0.3 and with $E_0\approx1.398$ being the ground-state energy. The latter agrees with the result $E_0=1.40\pm0.01$ of [12]. We found that both the data of [6] and our

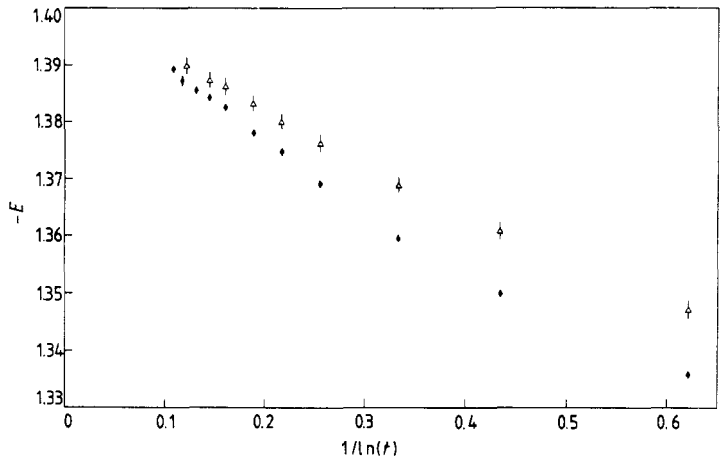

Figure 1. Energies of the 'ground states' reached after cooling with a rate $1/t$. In view of the ansatz (3), these energies are plotted against $1/\ln t$. △, data of [6] (100×100), ◇, our results (240×240). In our data, the statistical errors are in general smaller than the size of the symbols.

Table 1. The first column gives the inverse cooling rates t in updates per spin for each temperature (the temperatures were $T=1.2$, 1.06, 0.92, 0.78, 0.64, 0.50, 0, the lattice size was 240×240). The second column gives the number of runs with this cooling rate and the third column gives the energy per spin reached.

t	Number of runs	E
5	100	1.335 75 ± 0.000 24
10	50	1.349 90 ± 0.000 33
20	50	1.359 48 ± 0.000 29
50	20	1.369 14 ± 0.000 32
100	20	1.374 75 ± 0.000 55
200	30	1.378 06 ± 0.000 40
500	30	1.382 54 ± 0.000 43
1 000	40	1.384 28 ± 0.000 29
2 000	12	1.385 55 ± 0.000 49
5 000	4	1.387 28 ± 0.000 79
10 000	24	1.389 34 ± 0.000 37

data are better described by (2) if a larger value $x \approx 0.35$ is taken, which would then give $E_0 = 1.393 \pm 0.003$ for both data sets.

Alternatively, it was proposed in [13] that $E(t)$ converges as

$$E(t) = E_0 + \frac{\text{constant}}{(\ln t)^{\zeta}} \tag{3}$$

with some unknown exponent ζ. Indeed a fit at least as good as the above was obtained with $\zeta \approx 1$. For this reason, $E(t)$ is plotted against $1/\ln t$ in figure 1. The extrapolation to $t = 0$ now gives somewhat larger values:

$$E_0 = \begin{cases} -1.403 \pm 0.002 & \text{(this letter)} \\ -1.401 \pm 0.004 & \text{(see [6]).} \end{cases} \tag{4}$$

This is in perfect agreement with the value $E_0 = -1.4024 \pm 0.0012$ found in [5] by means of the transfer matrix method.

Both in [6] and in the present work, no finite-size corrections have been taken into account. We feel that we are reasonably safe due to the large lattice size (the lattices in [6] were only of size 100×100). One possible source of finite-size corrections specific to the present letter consists in our putting all horizontal bonds to $-J$. On a finite lattice, there is at most one bond per line which cannot be gauged ferromagnetic. The error in the ground-state energy committed thereby can be estimated exactly as $\leqslant |E_0|/2L \approx 0.003$. According to test runs on smaller lattices, it actually seems to be much smaller than that.

Summarising, we have presented Monte Carlo results of a new algorithm for the ground state of the two-dimensional $\pm J$ spin glass. It is not only very fast (indeed it seems the fastest algorithm in the literature), but it also uses very little storage. While it would not be straightforward to extend it to spin glasses with continuous distributions of bonds, the extension to three dimensions is trivial. Our numerical results improve the best previous Monte Carlo results. Their extrapolation to infinitely slow cooling agrees perfectly with the most precise results of a transfer matrix calculation [5], provided we use in this extrapolation the cooling rate dependence predicted in [13]. If we would use instead the power law conjectured in [6], our extrapolated value would disagree with that of [5] by around three standard deviations. Thus we conclude that both [5] and [13] are correct, and that a power law as proposed in [6] is ruled out.

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