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Replica optimization method for ground-state search of random spin systems

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Abstract. A new method to find ground states is proposed for random spin systems. It is applicable to systems with any boundary conditions, any bond distribution and any magnetic field. The efficiency of this method is confirmed numerically in the case of the two-dimensional Ising spin glass with Gaussian bond distribution in a uniform field. The introduction of more than two replicas improves the efficiency of the method considerably. It is also found that the renormalization process is effective. The increase in computational time with respect to system size is moderate and well fitted by a power law up to $L = 32$. Magnetizations are calculated for various magnetic fields using the new method. The size dependence of the susceptibility is found to be $\chi(L) \propto L^x$ with $x = 0.476(5)$. This is somewhat larger than predictions using domain-wall renormalization group arguments.

1. Introduction

For the last 20 years, random spin systems have attracted the interest of many physicists. This is because they are the simplest examples of random systems and models such as the Edwards–Anderson (EA) model and the SK model can be regarded as minimal models of random systems. Furthermore, the mean-field (SK) model has many interesting features. Several exotic concepts such as replica-symmetry breaking, metastability of the low-temperature phase, multi-valley structure and the ultrametric structure of the phase space are proposed in the course of the investigation of this model.

There is, however, some evidence [1, 2] and there have been discussions [3–6] which suggest that the nature of random spin systems in finite dimensions may be quite different from that of the SK model. The essential difference lies in the properties of the low-temperature phase. For example, Monte Carlo simulations for the $\pm J$ model in three dimensions [1] suggest that, even in the low-temperature region, the Edwards–Anderson order parameter q_{EA} tends to zero in the limit $t \to \infty$ and recent results of Monte Carlo simulations for the same model in the low-temperature region [7] show that the surface susceptibility converges to zero in the thermodynamic limit, indicating that $q_{\mathrm{EA}} = 0$. These facts can not be explained by the mean-field theory. The scaling theory [4, 5], based on the assumption that there are only two phases below the critical point, seems to be successful in explaining several aspects of finite-dimensional systems, and it predicts the absence of the phase transition in the presence of a magnetic field. In this theory we assume a situation similar to that described by

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the random ordered phase (ROP) picture which was originally proposed by Ueno and Oguchi [8]. The ROP is an ordered phase in which percolated non-frustrated clusters in the system exhibit a phase transition similar to that of the Mattis model. This picture is, however, incompatible with the above results which suggest that $q_{EA} = 0$.

In addition, a Monte Carlo simulation was recently performed for the $\pm J$ model in three dimensions in the presence of a uniform magnetic field [9]. According to it, the phase boundary seems to exist which corresponds to the AT line for the SK model, though the variance of the distribution function $P(q)$ converges to zero in the thermodynamic limit even in the ordered region. Another recent Monte Carlo simulation [10] shows that the contour of the constant spin-glass susceptibility does not seem to approach the line $H = 0$ and the existence of the AT line is insisted on. Hence the controversy concerning the nature of the ordered phase is far from being settled.

To investigate such subtle problems regarding these models, numerical methods are promising. The transfer-matrix method is one of the most powerful methods for calculating the exact ground states. The computational time, however, increases proportionally to $L^{\alpha}2^{(d-1)L}$ ($\alpha > 0$, L is the linear size of the system) and the memory storage required also grows exponentially. Nevertheless, there are some methods [11–13] by which one can obtain the free energy with a computational time proportional to $O(N^2)$, where N is the number of spins.

As for the investigation of the ground states, one can obtain the ground state within a time of the order of $O(N^3)$ [12, 14–17]. Unfortunately, these methods are available only to the two-dimensional system without magnetic field. Furthermore, it is proved that the problem of the ground-state search is NP-hard in the case of a non-vanishing magnetic field and for three or more dimensions. Generally speaking, the only method which enables us to study large systems is one which invokes random numbers, such as Monte Carlo simulation. This method, however, encounters the difficulty of the extremely long correlation time below T_c.

In the present paper we propose a new method for investigating the ground-state properties of such random systems. Strictly speaking, our procedure does not guarantee the exact ground state. It is shown, however, that we can find it with a remarkably high probability and in a reasonable computational time.

The present work is inspired by the replica Monte Carlo method [18] proposed by Swendsen and Wang and the new method presented in this paper can be regarded as its extension to the ground-state search. There are, however, two ingredients in the present method which Swendsen and Wang's algorithm does not share.

First, in the present method, more than two replicas are compared in the determination of clusters which are taken to be the units of updating, while only two replicas are compared in Swendsen and Wang's algorithm. The number of replicas is a key factor contributing to the efficiency of the algorithm, as discussed later. For example, if this number is too small, percolation of clusters takes place. In such a case we cannot find relevant clusters with small excitation energy but only find a union of many such clusters by comparing replicas. In the worst case, such an 'accidental' big cluster may contain almost all the spins in the system and, as a result, the method becomes ineffective. Swendsen *et al* reported [19] that this is also the main reason why their procedure does not work so well for systems in three dimensions as in two dimensions.

Second, we have taken into account the fact that the low-lying excitations have themselves a hierarchical structure or a scaling property, as discussed by Fisher and Huse [4, 5]. In our method, a clustering procedure is performed hierarchically in a

fashion similar to the renormalization transformation. By doing this, the efficiency of the method is greatly improved.

In section 2 we describe the method and in section 3 we show how effective it is for the two-dimensional EA model with a Gaussian bond distribution. In section 4 the magnetization is measured in the presence of a magnetic field and we find that the size dependence of the susceptibility can be given as $\chi(L) \propto L^{0.476}$. This relation leads to the scaling form $m(L)L = f_{\text{scaling}}(HL^{1.476})$, which implies $m \propto H^{0.678}$. From this result and Fisher and Huse's droplet theory we have $\theta \approx 0.476$, where θ is the exponent which characterizes the size dependence of the droplet-excitation energy. In section 5, some discussions and a summary are given.

2. The replica method

In general, it is difficult (NP-hard) [20, 21] to find the exact ground state of a random spin system with a given bond configuration. If we try to find the ground state using one of the standard methods such as simulated annealing (SA) or the transfer-matrix (TM) method, it takes at least a computational time proportional to $\exp(aN^b)$, where a and b are positive constants and N is the total number of spins.

In this section, we formulate an alternative method which is far more effective than the standard methods in several cases. If we try to find ground states of systems in finite dimensions by SA, difficulties arise from large-scale elementary excitations. Fisher and Huse [4, 5] discussed the scaling properties of such excitations extensively and they call such excitations droplets. Thus the problem which we have to solve here is how to find such excited clusters. If we find all the excited droplets for a spin configuration, we can get the exact ground state by flipping them.

Our starting point for this problem is the fact that many local frozen clusters of spins can be observed when a random spin system at sufficiently low temperature is simulated using a standard Monte Carlo technique, say the Metropolis algorithm with single-spin updating. It is quite natural that a close relationship exists between these clusters and the droplets. We can determine frozen clusters either by comparing two spin configurations which are separated by a long time interval, or by comparing two spin configurations independent of each other, which are constructed by starting from different initial states. Thus one can easily think of a naive method of optimization as follows.

(1) Generate two spin configurations ('replicas') using the standard Monte Carlo method at an appropriate temperature or using simulated annealing with a particular cooling schedule. (Let us denote them as $S^{(1)}(\boldsymbol{R})$ and $S^{(2)}(\boldsymbol{R})$, respectively. Here $S^{(\mu)}(\boldsymbol{R})$ takes the values $+1$ or -1 for each site $\boldsymbol{R}$.)

(2) Assign the number

$$(1 - S^{(1)}(\boldsymbol{R}) \times S^{(2)}(\boldsymbol{R}))/2 \tag{2.1}$$

to each site $\boldsymbol{R}$. (We call this integer a colour number of the site $\boldsymbol{R}$.) Then divide the whole system into clusters. Here, a cluster is a group of sites with the same colour which are connected to each other by bonds.

(3) If flipping of all the spins in a cluster lowers the energy we flip them, then we repeat this procedure for all the clusters.

It is possible that this naive optimization lowers the energy considerably. It cannot be expected, however, that such a single operation is enough to find the exact ground state. In order to obtain a more efficient method we must take into account the following two facts which we have ignored in the above naive optimization. First, because of the percolation of the clusters, the probability can be very small that an excited droplet is flipped. When all the cluster has percolated and as a result there is only one large cluster, the above procedure is clearly useless, because the resulting configuration is one of the two initial configurations $S^{(1)}$ and $S^{(2)}$. There is no improvement compared to the initial configurations in this case. This difficulty is more serious in higher dimensions, since the percolation threshold is lower in such situations.

Second, each spin belongs in general to many droplet excitations with different scales at the same time. Therefore, we cannot expect that all the clusters with different scales are optimized by only a single step of the replica optimization.

The first difficulty can be resolved by introducing many replicas, as we will see below. The second difficulty of the naive method can be cleared by introducing iterative operations of the replica optimization. There are several ways to achieve this. One can arrange single operations hierarchically while a one-dimensional arrangement is also possible. In the actual numerical calculations presented in sections 3 and 4, we have used the one-dimensional arrangement in the main.

Now, let us describe the elementary operation in which many replicas are included. In order to prevent the clusters from percolating, it is effective if we increase the number of colours which we introduced in the naive optimization for division of the system. The probability for two random clusters to have the same colour accidentally is diminished by doing so. The most desirable situation is that each cluster has a different colour from all the others. Taking these facts into account, we consider here the following elementary operation over n spin configurations. Let us call them replicas and denote them as $S^{(\mu)}(\boldsymbol{R})$ $(\mu = 1, 2, \ldots, n)$, as before.

(1) Initialization. Define vertices as follows:

$$v_i \equiv \{\boldsymbol{R}_i\} \qquad i = 1, 2, \ldots, N. \tag{2.2}$$

Assign a vertex variable $\sigma_v^{(\mu)}$ and a vertex magnetization μ_v to each vertex. Assign an inter-vertex coupling constant $J_{vv'}$ to each pair of two vertices. The initial values for these new variables are as follows:

$$\sigma_{v_i}^{(\mu)} \Leftarrow S^{(1)}(\boldsymbol{R}_i) \times S^{(\mu)}(\boldsymbol{R}_i)$$

$$\mu_{v_i} \Leftarrow S^{(1)}(\boldsymbol{R}_i)$$

$$J_{v_i v_j} \Leftarrow J_{ij}.$$

(2) Assign a 'colour number' to each vertex. The 'colour number' is an integer defined by the following equation:

$$\psi_v \equiv f(\sigma_v^{(1)}, \sigma_v^{(2)}, \ldots, \sigma_v^{(n)}) \equiv \sum_{\mu=2}^{n} 2^{\mu-3}(1 - \sigma_v^{(\mu)}). \tag{2.3}$$

This is a straight-forward extension of the previous definition (2.1) for $n = 2$.

(3) Divide the system into clusters.

(4) Assign a cluster variable $\tilde{\sigma}_c^{(\mu)}$ to each cluster in each replica as follows:

$$\tilde{\sigma}_c^{(\mu)} \Leftarrow \sigma_v^{(1)} \times \sigma_v^{(\mu)} \qquad (v \subset c). \tag{2.4}$$

Assign a cluster magnetization $\tilde{\mu}_c$ to each cluster as follows:

$$\tilde{\mu}_c \Leftarrow \sum_{v \subset c} \mu_v. \tag{2.5}$$

(5) Calculate the inter-cluster couplings $\{\tilde{J}_{cc'}\}$ which are defined as

$$\tilde{J}_{cc'} \equiv \sum_{\substack{v \subset c \\ v' \subset c'}} J_{vv'} \sigma_v^{(1)} \sigma_{v'}^{(1)}. \tag{2.6}$$

(6) Rename 'clusters' as 'vertices', i.e.

$$\sigma_c^{(\mu)} \Leftarrow \tilde{\sigma}_c^{(\mu)}$$

$$\mu_c \Leftarrow \tilde{\mu}_c$$

$$J_{cc'} \Leftarrow \tilde{J}_{cc'}.$$

(7) Change the sign of each new vertex variable on a replica if the energy is lowered by doing so. Repeat this procedure for all the vertices until there is no vertex to be changed. (Let us call these operations 'vertex-quench'.) Apply the vertex-quench to all the replicas.

(8) If all the replicas coincide, that is, if

$$\sigma_v^{(\mu)} = \sigma_v^{(\mu')} \tag{2.7}$$

holds for any μ, μ' and v, the elementary operation is terminated.

(9) If any change occurs during the last pass of step 7, go to step 13.

(10) Calculate the total inter-vertex energy

$$E^{(\mu)} \equiv -\sum_{vv'} J_{vv'} \sigma_v^{(\mu)} \sigma_{v'}^{(\mu)} - H \sum_v \mu_v \sigma_v^{(\mu)} \tag{2.8}$$

for each replica.

(11) Let μ_0 be the index of the replica which gives the minimum energy. Replace all the vertex variables except for those of the μ_0th replica by random numbers which take the values $+1$ and -1 with equal probability.

(12) Apply the vertex-quench to all the replicas except for the μ_0th replica.

(13) Change the sign of the original spin $S^{(1)}(\boldsymbol{R}_i)$ if

$$\boldsymbol{R}_i \in v \quad \text{and} \quad \sigma_v^{(1)} = -1. \tag{2.9}$$

(14) Go to step 2.

It can easily be seen that in the case of two replicas ($n = 2$) the two configurations coincide after the first pass through to step 7 and consequently that steps 8 to 14 are useless.

Repeated application of steps 2 to 7 is particularly effective in the case of the one-dimensional arrangement presented below. In this case, there is one special replica which has been optimized much better than the others. In other words, the optimized scale of the other $(n-1)$ replicas is smaller than the first one. The typical size of the clusters which appear at step 3 is determined by this optimized scale of $(n-1)$ replicas. Therefore, the probability is very small in general that an excited droplet is recognized as a single cluster if it is much larger than the typical size of these clusters. As a result, the energy of the first replica is hardly lowered by only one pass of steps 1 to 7 since most of excited droplets in this replica are much larger than the typical size. This difficulty can be partially overcome by optimizing the $(n-1)$ replicas as well as the first replica and by applying steps 2 to 7 repeatedly until all the replicas coincide.

Steps 10 to 12 may make the whole procedure more efficient, although they are not as crucial as the other part. In fact, the elementary operation works well without these steps, if a proper condition of termination is provided.

In order to explain the complete algorithm we have to describe how the above elementary operation is applied repeatedly. Although even a single elementary operation is effective in lowering the energy, for large systems one can hardly reach the exact ground state by only one operation. The simplest solution to this problem is to form a sequence of elementary operations. That is, the final spin configuration of the ith operation is used as one of n initial spin configurations for the $(i+1)$th operation and the other $(n-1)$ initial configurations are obtained by quenching spin configurations at $T = \infty$ (completely random configurations). In the following sections we use this type of arrangement.

There is an alternative choice in which there is no special initial spin configuration for each operation. That is, all the initial configurations for an operation are the final configurations of the other n operations which are independent of each other. This type of arrangement produces a tree-like structure. In this case, the number of total operations grows very rapidly as the number of generations is increased. In spite of this disadvantage, this type of arrangement may be necessary for treating very large excitations. We expect that this tree-like (hierarchical) structure is suitable for treating large droplet excitations, because the droplets have in general a hierarchical structure. Several droplets compose a large cluster, several large clusters compose a larger cluster, and so on. In order to separate a droplet of a particular scale from other parts of the system, all the initial spin configurations must be well optimized up to the scale of such a droplet. Otherwise it will be divided into pieces at step 3 in the elementary operation described above and therefore this operation will fail to recognize the droplet as a single cluster.

As we have already stated above, however, this difficulty is partially (or maybe completely) overcome by introducing the renormalization procedure realized by step 6 and by repeated applications of steps 2 to 7. We found that the hierarchical arrangement is not necessary at least for $L \leq 32$ where the one-dimensional arrangement is good enough, as we will see below.

3. Computational time and efficiency

In this section, we demonstrate the efficiency of the method described in the previous section in the case of the EA model on the two-dimensional square lattice with a Gaussian bond distribution. The distribution of the coupling J is given by

$$P(J) = (2\pi)^{-1/2} \exp(-J^2/2) \tag{3.1}$$

where we have adopted periodic boundary conditions. Calculations were performed for several bond samples. For each bond sample, we calculated eight sequences with different initial spin configurations in parallel. Calculations for all these sequences were stopped when the eight spin configurations coincided with each other. In order to avoid unnecessary optimization, if there is more than one sequence for which the energy is the lowest, calculations for such sequences are stopped until a lower energy is found in the other sequences.

In figure 1, we show the minimum energy $E_{\min}(t)$ as a function of the number of trials (t) for $L = 64$ and $H = 0$ for a single bond sample. The average was taken over sixteen independent runs for simulated annealing (SA) and the Monte Carlo quench method (MQM) and four runs for the present method (the n-replica optimization method (n-ROM)). The Monte Carlo quench method was adopted by McMillan [22] for calculating the ground states of the present model and it proved to be effective for small systems ($L \leq 8$). One sweep of the Monte Carlo updating over all spins is considered as one trial for SA and for the MQM. The scheduling of cooling for SA was determined empirically. We set the temperature as follows:

$$T(t) = a \exp(-4t/t_{\max}) + b \tag{3.2}$$

where a, b and $t_{\max}$ were determined so that $T(0) = 2.0$ and $T(t_{\max}) = 0.5$. The temperature used for the MQM was determined empirically as well. In fact, we studied at $T = 0.6$. We also tried other temperatures: 0.3, 0.4, 0.5, 0.7 and 0.8, and found that the value $T = 0.6$ is optimum for this system size and for $t_{\max} = 1024$. For this system size ($L = 64$) the exact ground state was not reached by any method within $t_{\max}$. Nevertheless, we can see from the figure that the n-ROM is faster than SA and the MQM. For example, the minimum energy reached by SA at $t = 1024$ was reached by 4-ROM at $t \simeq 3$. Of course, the CPU time per trial is longer for 4-ROM than for SA. This fact does not, however, change the superiority of the 4-ROM over SA, since the ratio of the CPU times per trial is no more than 30. We can also see from figure 1 that n-ROMs for $n > 2$ are more effective than 2-ROM, as we pointed out in the previous section. We can see this more clearly in figure 2 which shows the replica-number dependence of the CPU time τ required for finding ground states in the cases where $L = 6$ and 8. It is clear that 2-ROM converges much more slowly than 5- or 6-ROM. The latter gives the minimum τ. This is because 2-ROM fails to separate a droplet from a large percolated cluster. On the other hand, such percolation of the 'same-colour' droplets hardly occurs for 5- or 6-ROM, since the number of colours (2^4 or 2^5) is much larger than that for 2-ROM (2^1). It should be noted, however, that the efficiency is not improved, when we increase the number of the replicas above a certain number. We can explain this in a similar way. That is, the increment has no advantage once the number of replicas reaches a certain number at which almost all the relevant clusters are separated. In addition, the CPU time per elementary operation grows as the replica

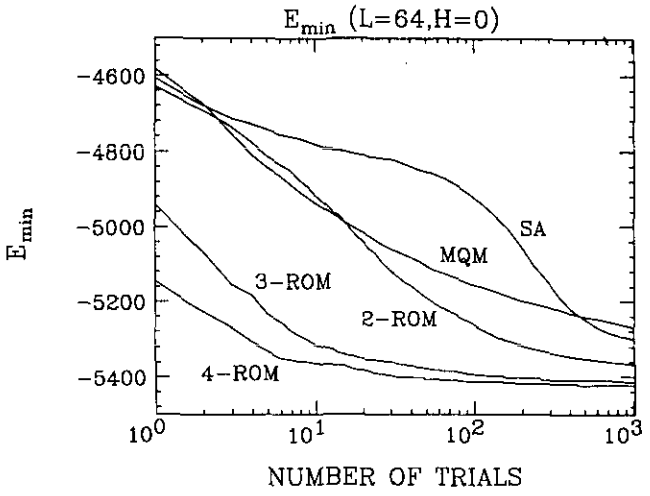

Figure 1. The lowest energy plotted against the number of trials for $N = 64 \times 64$. The symbols 'SA', 'MQM' and 'n-ROM'($n = 2, 3, 4$) stand for simulated annealing, the Monte Carlo quench method and the present method with n replicas, respectively. The scheduling of the simulated annealing is determined empirically by several trials. The temperature for the Monte Carlo quench method is $T = 0.6$ which is found to be optimum for this size. The unit of the horizontal axis is one sweep of Monte Carlo updating over all spins for SA and MQM and one elementary operation for n-ROMs.

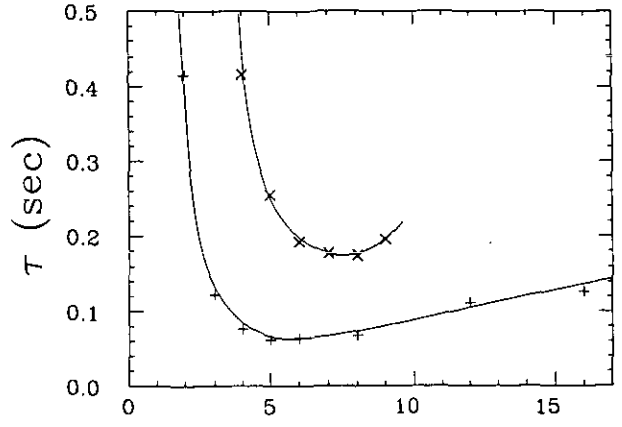

Figure 2. The average time required to find a ground state plotted against the the number of replicas for $L = 6$ (+) and $L = 8$ (×).

number increases. Thus the total efficiency is diminished for replica numbers that are too large. In table 1, the number of replicas we have used is listed, together with the average CPU time per ground state for $6 \leq L \leq 32$. The listed replica numbers are

Table 1. The first column (L) shows the system sizes and the second column (n) shows the number of replicas adopted for each system size in the present calculation. The number N_{sample} is the number of different bond configurations used in calculating the average CPU time (τ).

L	n	N_{sample}	τ (s)
6	6	128	0.064
8	7	128	0.17
10	8	32	0.68
12	9	32	1.5
16	10	32	7.3
20	12	32	23
24	14	8	44
32	20	4	260

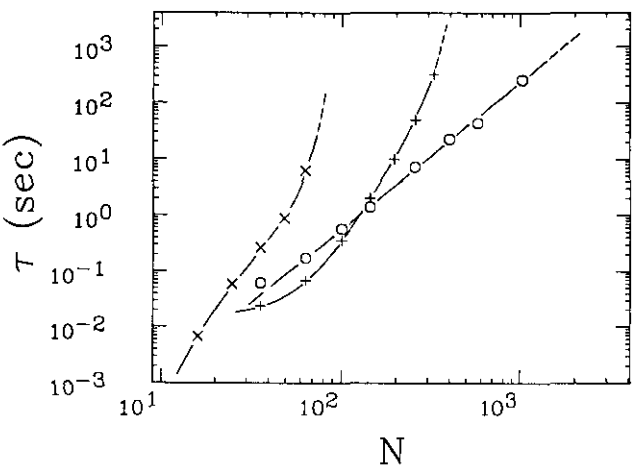

Figure 3. The average time required to find a ground state plotted against the system size. The different symbols correspond to different methods: the simulated annealing (x), the transfer-matrix method (+) and the present method (o). The curves are guide lines for eyes.

determined empirically and can be taken as approximate optimum numbers. It should be noted, however, that the CPU time for $n \pm 1$ is almost the same as that for n.

Figure 3 shows the averaged computational time (τ) plotted against the total number of spins (N). To be precise, τ is the time required for one of the eight sequences to reach the ground state averaged over the sequences and the bond configurations. It is easily seen that the present method is faster than the ordinary simulated annealing method for any N and faster than the transfer-matrix method for large N. In addition, it is remarkable that only τs for the present method are well fitted by the power law, i.e.

$$\tau \propto N^{\lambda} \qquad \lambda \sim 2.6. \tag{3.3}$$

Computational times for the other methods diverge more rapidly than the power law. However, it is necessary to perform the calculations for larger systems and folllow the analytical discussion to confirm the asymptotic power-law behaviour of the computational time.

Of course, the computational time depends on what machine is used to perform the calculation. All the numerical calculations presented here were performed on the VAX6440 of the Meson Science Laboratory at the University of Tokyo. Roughly speaking, however, the CPU time for other machines is proportional to that for the present machine, displayed in figure 3. Therefore, we believe that if the same calculation was performed on a different computer, a figure similar to figure 3 would result, and would be different from it only by the unit of the vertical axis as long as the relevant machine is a standard scalar computer.

If we use other types of computer, such as vector machines which accelerate some particular types of programs, the relative placement of three sets of data points in figure 3 will be changed. In practice, the present method is not suitable for vector processors because of the clustering procedure (step 3 in the elementary operation) while the other two methods can be vectorized completely. In addition, the Monte Carlo updating is accelerated by a factor of 10 to 100 by the multi-spin coding (for example, see [23, 24]), although it does not accelerate a single sequence of the Monte Carlo updating. Even if we take these facts into account, the present method is faster in finding the ground states than simulated annealing if $L \geq 12$. For $L \geq 12$ we could not find any exact ground state in reasonable computational time ($\tau < 10$ hours) by simulated annealing. The n-ROM is faster than the transfer-matrix method for the case $L \geq 16$ because the vectorization favours the transfer-matrix method only by a factor of 10 to 100. Furthermore, it should be noted that, for periodic boundary conditions, the transfer-matrix method requires much more time and memory than for open boundary conditions. In this case, the computational time and the memory storage needed in calculation are proportional to 2^{2L}. Therefore, it is almost hopeless to calculate a ground state for large systems, say for $L \geq 16$ in this case.

The effect of a homogeneous magnetic field on the computational time in our method is a subtle problem. It is obvious that if the field is strong, the ground state is almost the same as the 'all-up' state where only small fraction of spins directed down against the field, and there is no high barrier between the ground state and the 'all-up' state. In such cases, the convergence of the present method is expected to be very rapid, since a spin configuration generated by a mere quench is already close to the ground state and there is no large low-lying excitation which makes it difficult to reach the true ground state. In spite of these facts an increase of the computational time was, however, observed when a weak magnetic field was applied. Of course, there is a certain peak above which τ decreases, as it should. The field dependence of the computational time is shown in figure 4 for $L = 6$ and $L = 8$.

We have checked that the states obtained by the present method are the true ground states by comparing those with the results of the transfer-matrix method for $L = 8$ and $L = 16$. We have calculated the ground states of 100 different systems with periodic boundary conditions in the case where $L = 8$. In the case where $L = 16$, we have examined 100 systems with open boundary conditions. In both cases we have performed our calculations for $H = 0$ and $H = 0.1$. Two sets of results obtained by different methods coincided with each other completely. For further confirmation, we compared two sets of results obtained by the present method with different replica numbers for periodic boundary systems with linear size $L = 16$. In this case, we detected one failure among 100 samples. Therefore, we can expect that the ratio of failures is very small and that it is approximately 1% at most. Thus these failures do not change our results in this paper beyond statistical error bars, at least for $L \leq 16$. We believe that this is also the case with the data for $L = 20$ and 24 presented in

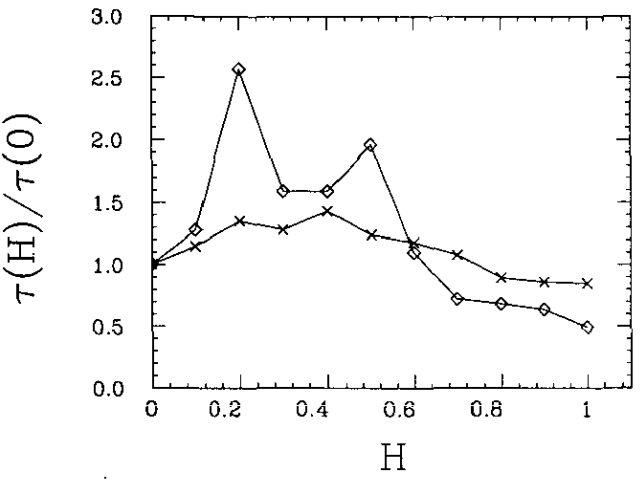

Figure 4. The average time required to find a ground state plotted against the magnetic field. The crosses (×) and the diamonds (◇) indicate data for $L = 8$ and $L = 12$, respectively.

the next section. In addition, we can in general diminish the fraction of failures by increasing the number of the parallel sequences if necessary.

4. Magnetization at $T = 0$

In this section, we apply the n-ROM to the EA model with a symmetric Gaussian bond distribution in the presence of a uniform field, and study the critical behaviour of the magnetization near $H = 0$ by means of the finite-size scaling method. Many authors have reported on this problem. For example, two-dimensional systems with continuous bond distributions are investigated in [25–27] (Gaussian bond distribution) and in [28] (rectangular bond distribution). The critical behaviour, however, is investigated mainly by calculations of the domain-wall energy. The stiffness exponent θ which characterizes the size dependence of the domain-wall energy is calculated directly in this method. The other critical exponents are derived using the domain-wall renormalization group (DWRG) argument [25, 29] with the estimated value for this exponent. In contrast, there are only a few direct estimations [27, 28] of other exponents such as γ, δ and ν and the precision of these direct estimations is not so good as that of the indirect one by DWRG arguments. Therefore, it is interesting to estimate directly critical exponents other than the exponent θ to see how good the indirect estimation is.

Using the transfer-matrix method at $T = 0$ the stiffness exponent θ has been estimated as $\theta = -0.281(5)$ [25] or $\theta = -0.291(2)$ [26] for the two-dimensional EA model with a Gaussian bond distribution. The DWRG argument and the scaling argument based on the droplet picture [4] yield the following scaling relations:

$$\nu = -\frac{1}{\theta} \tag{4.1}$$

and

$$\delta = 1 - \frac{2\theta}{d}. \tag{4.2}$$

Here ν and δ are defined in the following asymptotic behaviours:

$$\xi(T) \propto T^{-\nu} \tag{4.3}$$

$$m(H) \propto H^{1/\delta} \tag{4.4}$$

where $\xi(T)$ is the correlation length and $m(H)$ is the magnetization per spin at $T = 0$. Substituting the estimated values into (4.1) and (4.2), we get

$$\nu = 3.6(1) \quad [25] \qquad \nu = 3.4(1) \quad [26] \tag{4.5}$$

and

$$\delta = 1.281(5) \quad [25] \qquad \delta = 1.291(2) \quad [26]. \tag{4.6}$$

On the other hand, the direct estimation of the exponent ν by the transfer-matrix method at finite temperatures [28] yields the following value for the exponent ν, somewhat smaller than the above results,

$$\nu = 3.0(2). \tag{4.7}$$

In this section, we assume the following scaling form for the magnetization per spin at $T = 0$:

$$\hat{m}(H, L) = L^{-\phi} \tilde{m}(HL^{\delta\phi}) \tag{4.8}$$

where

$$\hat{m}(H, L) \equiv m(H, L) - \lim_{H \to 0^+} m(H, L) \tag{4.9}$$

and $\tilde{m}(x)$ is a scaling function. The scaling form (4.8) implies that

$$m(H) \equiv \hat{m}(\infty, H) \propto H^{1/\delta} \tag{4.10}$$

$$\chi(L) \equiv \lim_{H \to 0} \frac{\hat{m}(L, H)}{H} \propto L^{\phi(\delta - 1)}. \tag{4.11}$$

We have calculated the magnetization per spin in various magnetic fields and for various system sizes in order to investigate the critical behaviour. The sizes of the systems we have treated for this purpose are $L = 6$ to $L = 20$, and the numbers of bond samples used for averaging are 1024 for $L = 20$ to 8192 for $L = 6$. The scaled data are shown in figure 5. In figure 5, we have adopted the value 1.0 predicted by the DWRG argument for the exponent ϕ and the value 1.476 estimated below for the exponent δ. From these data we have estimated the susceptibility for each system size. In this estimation, only data for sufficiently small fields are used to avoid the effect of terms with higher orders in H. In figure 6, the size dependence of the susceptibility is shown. Least squares analysis to the present data results in

$$x = 0.476(5) \tag{4.12}$$

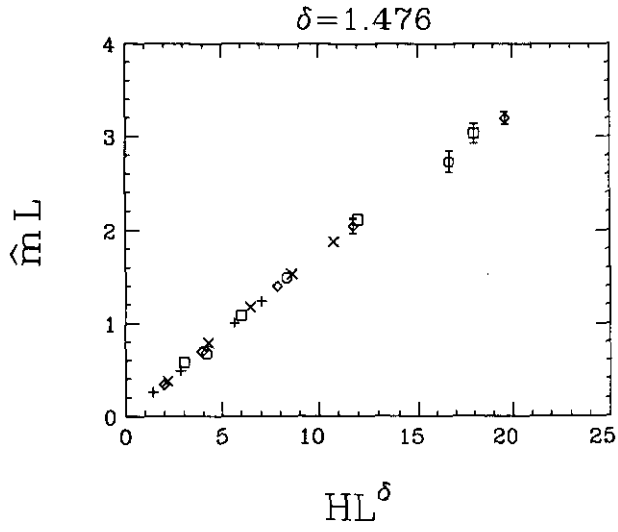

Figure 5. The scaling plot of the magnetization. The scaled variables are $HL^{\phi\delta}$ and $\hat{m}L^{\phi}$ with $\phi = 1$ and $\delta = 1.476$. Symbols stand for $L = 6$ (+), 8 (×), 12 (◇), 16 (□) and 20 (○), respectively.

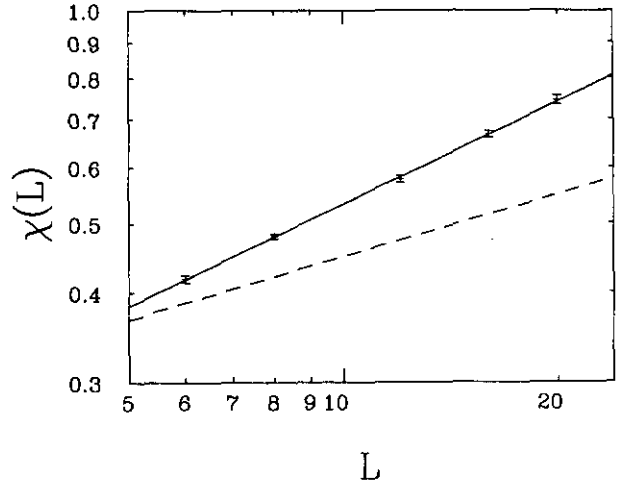

Figure 6. The size dependence of the susceptibility $\chi(L)$. The straight line is the result of a least squares analysis with the fitting function $\chi(L) = aL^{x}$ which yields $x = 0.476$. The broken line indicates the inclination predicted by the DWRG argument ($x = 0.291$).

when we use a simple fitting function

$$\chi(L) = aL^{x}. \tag{4.13}$$

According to the DWRG argument, the above exponent x is directly related to the stiffness exponent θ by the following equation:

$$x = -\theta. \tag{4.14}$$

Since there are no critical exponents other than x and θ in the above equation, it is convenient to compare our result with the prediction of the DWRG arguments by calculating this exponent. Our estimation (4.12) is clearly larger than the DWRG prediction beyond the statistical error. In order to eliminate a possible finite-size effect more carefully, we have tried another fitting function for our data. That is, we have added an extra constant to the system size L as a fitting parameter. Then the new fitting function becomes

$$\chi(L) = a(L+b)^x. \tag{4.15}$$

In this case, the resulting value of the exponent x is

$$x = 0.51(4). \tag{4.16}$$

Again, our result is not compatible with the DWRG prediction. The exponent ϕ is predicted to be unity by the DWRG argument. If this is the case, (4.12) produces

$$\delta = 1.476(5). \tag{4.17}$$

This is the value used in the previous scaling plot in figure 5.

At present, we have no complete explanation of the discrepancy between our result and the DWRG argument based on the numerical estimation of the stiffness exponent.

5. Discussion and conclusions

In this paper we have presented a new method to calculate the exact ground states for two-dimensional systems in several conditions which are not tractable by the ordinary transfer-matrix method, the simulated annealing method or methods based on graph theory and the theory of linear programming. The present method is also effective in calculations for large systems without a field. We have demonstrated that the introduction of many replicas improves the efficiency remarkably. This is because undesirable percolation of clusters takes place for small n and it prevents effective flipping of large excitations, whereas with many replicas each relevant excitation can be recognized separately. It has been confirmed numerically that our method works well, at least, for system size $L \leq 32$. The size dependence of the computational time is moderate and well fitted by the power law

$$\tau \propto N^{2.6} \tag{5.1}$$

for $N \leq 1024$. Thus, the present method is found to be promising even for larger systems. In addition, the present method works also in the presence of uniform field. This method is simpler than other methods based on the theory of linear programming, and the physical meaning of it is clearer. Formally, it is applicable to problems in dimensions higher than three, although its efficiency has not been checked. Furthermore, it should be noted that the present method can be generalized to study finite-temperature properties. That is, we can easily construct a new replica Monte Carlo algorithm with more than two replicas. We expect that the introduction of many replicas resolves the difficulty that arises from the percolation of relevant excitations

[19] and that we may overcome the long-relaxation time even in three dimensions. The detail of this extension of the n-ROM will be presented in the near future.

Of course, since the problem in the non-zero uniform field belongs to the class of NP-complete problems, some 'bad' bond samples exist for which convergence takes far longer than for other samples of the same size. The fraction of such 'bad' samples for which convergence takes more than ten times longer than the average is small, say 10% at most, in every case we have investigated so far. How to diminish this fraction and how to treat 'bad' cases are interesting future problems.

The physical result presented in section 3 is somewhat peculiar. It suggests that the DWRG argument with the numerical estimations of the stiffness exponent fails to predict the value of the exponent δ precisely. It is important to clarify whether the discrepancy between our result and the previous results is due to the finite-size effect or to wrong assumptions in the DWRG argument. Unfortunately, we do not have an objective and reliable criterion to determine whether certain data lie in the critical region or not. The only method available to us is to see how well the scaled data can be fitted by a particular curve. It cannot help being more or less subjective. Thus we cannot in general exclude the possibility that the finite-size effect may have affected our estimation of the critical exponents. In the present case, however, our data for the susceptibility obey the power law

$$\chi(L) \propto L^{x} \qquad \text{with } x = 0.476(5) \tag{5.2}$$

very well. The chi-square divided by the degree of freedom (= 3) is 0.21 in the least squares analysis with a trial function (4.13). Hence, it is natural to assume that the behaviour remains the same for systems larger than the ones we have investigated. On the other hand, the data which were used in the estimation of the stiffness exponent [26] seem to be fitted by a power law very well. Thus it is also natural to expect that the true value of the stiffness exponent does not lie far beyond the statistical error. If this is the case, the reason for the discrepancy that we have observed must be looked for in the DWRG argument. For example, the discrepancy can be explained by assuming that the stiffness exponent which characterizes the size dependence of the domain-wall energy does not coincide with the exponent which characterizes the size dependence of the droplet excitation energy, although we have not expected such a situation.

In any case, our result shows that we have to be careful in estimating the critical exponents in an indirect way using the DWRG argument. We believe that the true critical behaviour of the present model will be clarified by direct estimations of critical exponents such as δ and γ in a finite magnetic field or at finite temperatures.

It should be mentioned that an analysis of the two-dimensional EA model with $\pm J$ bond distribution by the present method is also an interesting problem since it belongs to a different universality class from that of the present system. The problem of whether the ground states for $\pm J$ distribution are paramagnetic or critical has not yet been settled. A recent numerical study [30] by the transfer-matrix method indicates exponential decreasing of the domain-wall energy ΔE with respect to the longitudinal length of the system.

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