A New Algorithm for the Monte Carlo Simulation of Spin-Exchange Kinetics of Ising Systems

ABDULLAH SADIQ*

Institut für Festkörperforschung der Kernforschungsanlage Jülich, D-5170 Jülich, West Germany

A new algorithm is described for the Monte Carlo simulation of spin-exchange kinetics of Ising model on a square lattice with nearest- and next-nearest-neighbor interactions. For sampling the equilibrium ensemble of such a system at 50% concentration this algorithm is as efficient as the standard algorithm at about $T/T_c = 0.78$ for a 40 × 40 lattice and at about $T/T_c = 0.70$ for a 80 × 80 lattice. At lower temperatures its efficiency rapidly increases, while at lower concentrations one has to go to still lower temperatures before this algorithm becomes as efficient as the standard algorithm. For the domain growth studies this algorithm is orders of magnitude less efficient than the standard algorithm during the initial phases of the time evolution of such systems quenched from high temperatures to below their critical temperatures. For quenches to $T/T_c = 0.34$ at 50% concentration the present algorithm becomes as efficient as the standard algorithm after about 1000 MCS (Monte Carlo steps/particle) for a 40 × 40 lattice and after about 3000 MCS for a 120 × 120 lattice.

I. INTRODUCTION

The Monte Carlo computer simulation method has evolved into a powerful tool for studying the equilibrium and transport properties and the approach towards equilibrium of physical systems [1]. The model system most extensively used in such studies is the Ising lattice gas described by the Hamiltonian [2]

$$H - \sum_i \mu_i n_i = - \sum \phi_{ij} n_i n_j + - \tag{1}$$

where μ_i is the chemical potential, ϕ_{ij} is the pairwise interaction parameter and n_i is the occupation variable associated with the ith lattice site such that $n_i = 1$ if the ith site is occupied and it is zero otherwise. The sum is taken over all the pairs of particles with non-zero ϕ_{ij}.

In order to study the dynamics of the configurations of such a system, one further assumes that its particles are in thermal contact with a heat bath which induces spontaneous transitions in the system. The probabilities of such transitions, among other things, depend on the temperature, T, of the heat bath and the energy changes,

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* Alexander von Humboldt Fellow. Permanent address: Pakistan Institute of Nuclear Science and Technology, P. O. Nilore, Rawalpindi, Pakistan.

δH, involved in these transitions. In the case of the particle-hole exchange (Kawasaki) dynamics of interest to us here such a transition probability which is consistent with the detailed balance condition may be written as [2, 3]

$$\tau_s W(n_i \to n_{l_i}) \frac{n_i}{c} (1 - n_i) = \frac{\exp(-\delta H/k_B T)}{1 + \exp(-\delta H/k_B T)} \frac{n_i}{c} (1 - n_{l_i}). \qquad (2)$$

Here τ_s is an undetermined time constant which we put equal to unity by measuring time in Monte Carlo steps/particle (MCS), k_B is the Boltzmann constant and c is the concentration of the system.

In the standard Monte Carlo algorithm one generates new configurations as follows [1, 4]. (i) An occupied site, i, and its nearest-neighboring site, l_i, are chosen at random. (ii) When l_i is empty then the energy required to move the particle into the empty site, δH, is calculated, otherwise the move is rejected and a new pair of sites is similarly chosen. (iii) A random number, R, uniformly distributed between zero and unity is chosen, and the particle is moved into the empty site, l_i, when R is less than the transition probability, W, given by Eq. (2).

For temperatures below the critical temperature of the system the probability of a successful move, P_s, sharply decreases with temperature (Fig. 1), resulting in the rejection of most of the attempted moves, and thus a lot of the computer time is wasted in attempting unsuccessful moves. In order to avoid such a waste of computer time, Bortz *et al.* [5] proposed an efficient Monte Carlo algorithm for the spin-flip- (Glauber-) dynamics of Ising systems. In their study of the time evolution of binary
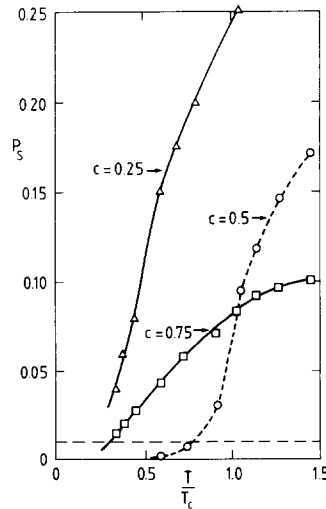

FIG. 1. Probability of a uccessful move, P_s, as a function of temperature, T, for a square Ising lattice gas with equal nearest- and next-nearest-neighbor repulsions for various concentrations as indicated in the figure. T is normalized by the critical temperature T_c approximate for $\Theta = 0.5$.

alloys they also made use of an algorithm which was intermediate between their new algorithm and the standard algorithm [6].

Here we describe a new algorithm for the Monte Carlo simulation of an Ising system on a square lattice with nearest- and next-nearest-neighbor interactions. In this algorithm bonds are randomly chosen only from "active bonds" (i.e., bonds joining nearest-neighboring occupied and empty sites) and the particles are always moved. The time is appropriatedly updated so as to make the results of this algorithm consistent with those of the standard algorithm. The details of this algorithm are described in Section II. In Section III we present some results for sampling the equilibrium configurations and for the approach towards equilibrium of such a system. Finally, in Section IV, we give our conclusions and comment on the range of applicability and possible extensions of this algorithm.

II. METHOD

II.1. The Bond Algorithm

The emphasis in the standard algorithm for the Kawasaki dynamics is on the sites of the lattice and may, therefore, also be referred to as the site algorithm (or SA). In contrast, the emphasis in the present algorithm will be on the bonds of the lattice and we will, therefore, also refer to it as the bond algorithm (or BA).

Since a square lattice of N sites has $2N$ bonds we assign two bonds to each lattice site, an x- and a y-bond. These bonds are classified into active and inactive bonds, where active bonds joining occupied sites with nearest-neighboring empty sites. Except for updating purposes, inactive bonds will be ignored in BA. For an Ising lattice gas on a square lattice with *equal* nearest- and next-nearest-neighbor interactions, the energy required to move a particle at the ith site to a nearest-neighboring empty site, l_i, is, modulo sign, given by (see Fig. 2)

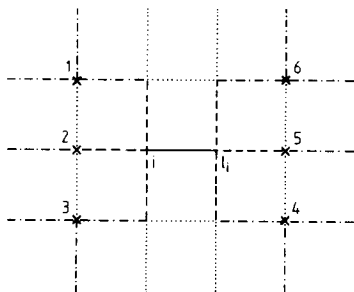$$\delta H = 2xI_2 = 4x[n_1 + n_2 + n_3 - (n_4 + n_5 + n_6)],$$

FIG. 2. The neighborhood of a bond which has been randomly chosen (——), along with bonds not affected by the move (···), bonds for which both activities and energies need to be updated (———) and bonds for which only energies need to be updated (· — · —).

or

$$I_2 = 2x[n_1 + n_2 + n_3 - (n_4 + n_5 + n_6)].$$ (3)

The energy index, I_2, given by Eq. (3) is a priori calculated for each bond. Since $-6 \leqslant I_2 \leqslant 6$, a factor of 20 is arbitrarily added to I_2 corresponding to inactive bonds,

$$I_2 \rightarrow I_2 + 20,$$

so that $I_2 > 6$ for these bonds. This fact is subsequently used to distinguish between active and inactive bonds. An array Iz is used for storing the particle (spin) configurations of the system and arrays IHx and IHy are used for storing the energy indices of x- and y-bonds, respectively.

Active bonds are grouped in seven classes, where the class index I_1 is related to its energy index, I_2, by the simple relation

$$I_1 = (I_2 + 8)/2.$$ (4)

The number of x- (y-) bonds in each class is stored into the array E (F) and these active bonds are labelled starting from bonds with the smallest class index (i.e., $I_1 = 1$). These labels are stored into an array LBx (LBy) and the x- and the y-coordinates of a bond of a given label are stored into arrays IKp, ILp (IKo, ILo), respectively. Thus given a label one can locate the coordinates of a bond and vice versa.

New configurations of the system are generated by randomly picking a bond from among the active bonds of the system and interchanging the empty and occupied sites across it. In order that new configurations in BA are chosen with the same a priori probability as those in SA seven numbers are calculated for each one of the seven classes of the x- (y-) active bonds as follows:

$$P_i = \sum_{j=1}^{i} E_j \times W_j$$

$$\left[Q_i = \sum_{j=1}^{i} F_j \times W_j \right]$$ (5)

where W_j is the transition probability of the jth class given by Eq. (2). A random number, R, uniformly distributed between 0 and $(P_7 + Q_7)$ is then chosen. For $R > P_7$ the active bond chosen is the y-direction, otherwise it is in the x-direction. The same random number, R, is also used to calculate the class index (and therefore the energy index) as well as the specific label, L, of the chosen bond. For, if

$$P_{i-1} < R \leqslant P_i,$$

then

$$I_1 = i, \qquad I_2 = 2I_1 - 8,$$

and

$$L - 1 = \begin{cases} (R - P_{i-1})/W_i, & I_1 > 1 \\ R/W_i, & I_1 = 1. \end{cases}$$

II.2. *Updating Energy Indices, Labels and Activities of Bonds*

Interchanging particle and a hole across an active bond, in addition to changing its energy index and consequently its label, may also change the activities, energy indices and labels of its neighboring bonds. For the system under consideration, there are 30 such neighboring bonds (Fig. 2). For the specific case of an Ising lattice gas with equal nearest- and next-nearest-neighboring interactions in which we are interested, 10 of these bonds (dotted lines in Fig. 2) are not affected by such a move. The bond which has been randomly picked (dark line in Fig. 2) remains active after the move, only its energy and label needing to be updated. For the six neighboring bonds touching this bond (dashed lines in Fig. 2) both the spin configuration and the energy change. Those of these bonds which were inactive become active and vice versa. The bonds which become inactive are removed from the list of active bonds and those which become active are included in this list with their specific energy indices and labels. For the rest of the 14 bonds which are not touching the chosen bond (dash-dotted lines in Fig. 2) only the energy indices are affected by the move. In this case, therefore, the activity of the bonds is not affected, and only the energy indices and the labels of the active bonds among these need to be updated.

II.3. *Time Scale*

A crucial element for BA, as indeed for the new algorithm of Bortz *et al.* [5], is the proper definition of the time scale. In the lattice gas version of SA, time is defined in Monte Carlo steps per particle (MCS), so that during such a unit of time each particle in the system, on the average, has a chance to move once. If N_p is the number of particles in the system and P_s is the probability of a successful move, then there will be, on the average, $N_p P_s$ successful moves during this unit of time. In other words, on the average, there is one successful move during every $1/(N_p P_s)$ MCS. In BA, on the other hand, every attempted move is a successful move. The time scale in this algorithm may, therefore, be made to correspond to that of SA by advancing it by an amount

$$\Delta t = \frac{1}{N_p P_s}, \tag{6}$$

MCS after every move. Also since in the SA bonds were chosen from among N_p out of the ZN_p possible bonds, Z being the coordination number of the lattice, while in the present algorithm bonds are chosen from among the N_B active bonds. Rescaling Δt by the ratio of these two numbers, we get

$$\Delta t = \frac{Z}{N_B P_s}. \tag{7}$$

At zero temperature the definition of active bonds is further restricted because at this temperature only those moves are allowed which do not increase the total energy of the system.

From Eq. (2) one may write

$$P_s = vW$$

where v is the vacancy availability factor, i.e., the probability of finding a vacant site which is nearest neighbor of an occupied site, and W is the transition probability of moving a particle from an occupied site into such a vacant site. In Eq. (7) the local instantaneous values of both v and W as well as the instantaneous value of N_B will be used. At very low temperatures this will give rise to large fluctuations in Δt due to the occasional but random choices of bonds with very small values of P_s. These fluctuations can be smoothed out by replacing W in Eq. (7) by its instantaneous average value given by [see Eq. (5) [5]],

$$\bar{W} = \frac{P_7 + Q_7}{ZN},$$

so that

$$\Delta t = \frac{Z^2 N}{N_B v (P_7 + Q_7)}. \tag{8}$$

III. Results

To explore the conditions under which BA is more efficient than SA parallel runs were made with two programmes which were identical, except that in one case configurations were generated with SA while in the other case these were generated with BA. Also, in view of the phase diagram of the system under consideration (Fig. 3) the equilibrium ensemble of this system was sampled at 50% and at 25% concentration at temperatures below the critical temperatures at these two concentrations.

Each successful move in BA involves updating the energies and labels of 21 bonds, while updating the label of a bond itself involves about $\frac{1}{2}N_B P_s$ operations. Also, since the time in BA increases inversely as P_s, we expect BA to be as efficient as SA for values of P_s given by

$$P_s \simeq \frac{1}{\sqrt{10 N_B}} = \frac{1}{\sqrt{10 Z v N_p}} \tag{9}$$

so that at 50% concentration one gets $P_s \simeq 1/\sqrt{10N}$, N being the lattice size. For a 40×40 lattice we get $P_s \simeq 0.008$, corresponding to $T/T_c = 0.75$ (see Fig. 1). The results of our calculations for the relative efficiency of BA compared to that of SA, t_B/t_S, for sampling the equilibrium configurations 40×40 and 80×80 lattices
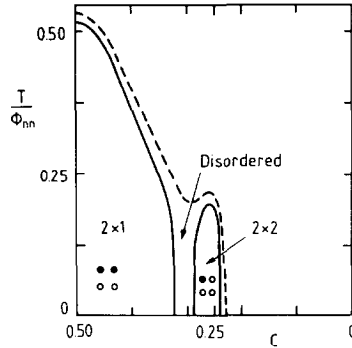
FIG. 3. Part of the phase diagram of a square Ising lattice gas with equal nearest- and next-nearest-neighbor repulsions (from Ref. [9]).

are given in Fig. 4. At 50% concentration BA becomes as efficient as SA at $T/T_c \simeq 0.78$ and at $T/T_c \simeq 0.7$ for these two lattice sizes consistent with Eq. (9). At 25%, the corresponding temperatures are $T/T_c = 0.29$ and $T/T_c = 0.15$, respectively.

For studying the domain growth of quenched systems the initial time evolution of the system after its disordered phase was quenched into its ordered phase was done with SA. The subsequent time evolution of the system after P_s had evolved to values smaller than the values given by Eq. (9) (see Fig. 5) was done with BA. This calculation was carried out to check not only the relative efficiency of BA but also to check the consistency of the definition of time given by Eq. (7). The results of this calculation for the time evolution of the energy for 80×80 and 120×120 lattices at $T/T_c = 0.6$, 0.34 and 0.0 are shown in Fig. 6. In this figure, the open symbols refer to the results obtained with BA and the solid symbols correspond to the results obtained with SA. The continuity of the points from SA into BA seen in this figure illustrates that the definition of time being used in BA (Eq. (7)) is consistent with that of SA.
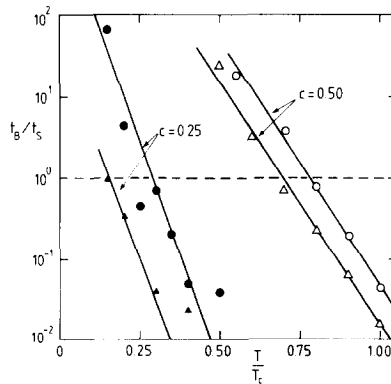

FIG. 4. Relative efficiency of bond algorithm compared to the site algorithm as a function of temperature for 40×40 (circles) and 80×80 (triangles) lattices at 50% and 25% concentrations. The two algorithms are equally efficient along the dotted line while solid lines are drawn to guide the eye.
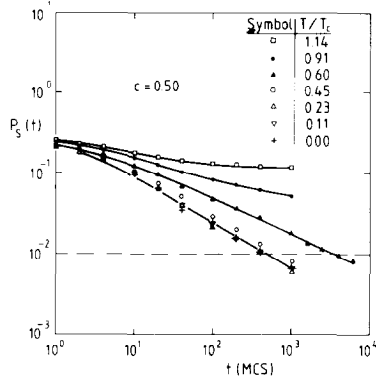
FIG. 5. Probability of a successful move, $P_s(t)$, as a function of time in Monte Carlo steps/particle after a high-temperature state of the system is quenched below its critical temperature at 50% concentration. The dashed line indicates the value of P_s for which the bond algorithm becomes as efficient as the site algorithm for a 40×40 lattice. The solid lines are drawn to guide the eye.

As is evident from Figs. 1 and 5, the use of BA in domain growth studies will helpful only at temperatures lower than $T/T_c \simeq 0.5$, after evolving the system with SA for several thousand MCS. The use of BA at $T/T_c = 0.6$, for a 120×120 lattice, for example, is only about 60% as efficient as that of SA after the system had been evolved with SA for 4000 MCS (see Fig. 6a). At $T/T_c = 0.34$, on the other hand, BA is 10–15 times as efficient as SA (Fig. 6b). The relative efficiency of BA at zero temperature is again somewhat lower as at this temperature the system freezes in metastable configurations and it does not seem to evolve towards its ground state.
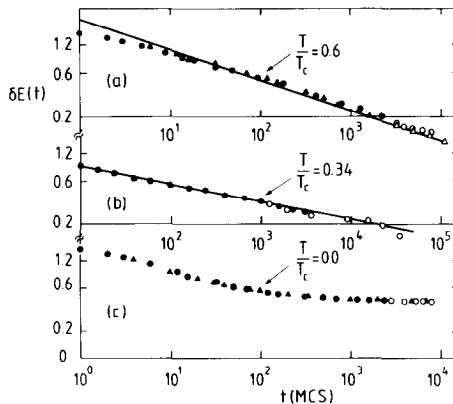

FIG. 6. Evolution of energy, $\delta E(t) = E(t) - \langle E \rangle$, with time, t, after the system is quenched from high temperature to below its critical temperature at 50% concentration for 80×80 (triangles) and 120×120 (circles) lattices. Open symbols are data taken with the bond algorithm and solid symbols are data taken with site algorithm. The temperatures to which the system is quenched are shown in the figure. The solid lines are taken from Ref. [8]. The relative efficiencies of the bond algorithm, t_B/t_s, for the (80×80) and (120×120) lattices, respectively, are (a) 2.0, 0.5, (b) 10.0, 15.0 and (c) 2.0, 0.74.
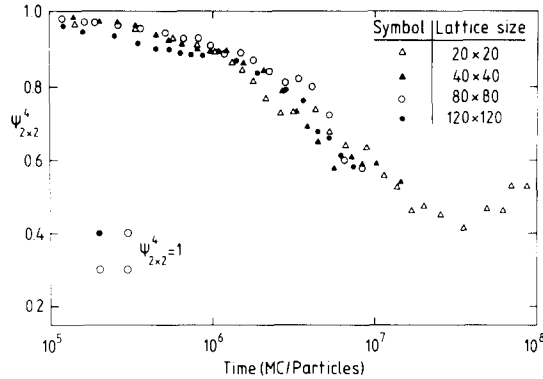
FIG. 7. Order parameter a (2×2)-structure as a function of time for 20×20, 40×40, 80×80 and 120×120 lattices at $T/T_c = 0.22$ and $c = 0.25$.

The bond algorithm could also be used for studying the stability of very low-temperature phases against thermal fluctuations. Such a study may be of some help to clarify the nature of some low-temperature phases, e.g., the nature of the phase at 0.25% concentration below $T/T_c = 0.45$ in the system under consideration, which is still not quite clear [7]. This can be done by starting with a possible ground state phase of the system at the concentration of interest and then studying the stability of this phase at various temperatures in the relevant part of the phase diagram. Preliminary results of such a study for (2×2)-phase at $T/T_c = 0.22$ are shown in Fig. 7. As is evident from this figure, such a study with SA would be prohibitively time consuming.

IV. CONCLUSIONS

The bond algorithm described in this paper should be very helpful for studying the static and dynamic aspects of Ising lattice gases and similar systems (Potts models, etc.) which manifest themselves at very low temperatures and/or very high densities. For example, apart from studying the nature of the low-temperature phases in some of these systems mentioned in the last section, this algorithm would also be very useful in further illuminating the structure observed in the tracer and collective diffusion coefficients of adsorbed monolayers at very low temperatures [2]. Its application in domain growth studies, though somewhat limited, can still be very helpful in deep quenches and in quenches close to the higher density phase boundary. The use of such an algorithm will be particularly helpful for studying Ising lattice gases where atoms tend to cluster together in the ordered phase, since in this case the drastic reduction in the vacancy availability factor will further enhance the relative efficiency of this algorithm. We emphasize that although the efficiency of the present

algorithm decreases with increasing system size (as more and more time is spent in updating the classification scheme of the active bonds), it still is orders of magnitude quicker than the standard algorithm in some cases of interest.

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