On the implementation of the 'heat bath' algorithms for Monte Carlo simulations of classical Heisenberg spin systems

1986 J. Phys. C: Solid State Phys. 19 2539

(http://iopscience.iop.org/0022-3719/19/14/020)

J. Phys. C: Solid State Phys. 19 (1986) 2539–2546. Printed in Great Britain

On the implementation of the 'heat bath' algorithms for Monte Carlo simulations of classical Heisenberg spin systems

Y Miyatake†, M Yamamoto‡, J J Kim‡, M Toyonaga§ and O Nagai‡
† Nippon Electric Corp, Kawasaki, Kanagawa 213, Japan
‡ Department of Physics, Faculty of Science, Kobe University, Rokkodai, Kobe 657, Japan
§ Matsushita Electronics Corp, Nagaokakyo, Kyoto 617, Japan

Received 28 October 1985

Abstract. The Monte Carlo simulations based on the 'heat bath' algorithms are implemented for the following classical spin systems: (i) the continuous-spin Ising model; (ii) the XY model; and (iii) the Heisenberg model.

1. Introduction

The Metropolis method of Monte Carlo (MC) simulations has been successfully applied to various Ising spin systems (see Binder (1984) and references therein). This method has also been utilised for classical Heisenberg spin systems (Binder 1976, Fernandez and Streit 1982, Teitel and Jayaprakash 1983). On the other hand, the 'heat bath' method, which is common for various lattice gauge models (Källe and Winkelman 1982, Rebbi 1984), has not yet been applied to the classical Heisenberg spin systems, as far as we know. In this paper, we report on the MC calculations based on the 'heat bath' algorithms for the classical spin systems.

2. Algorithms

Let us assume n local-energy levels, $(\varepsilon_1, \varepsilon_2, \ldots, \varepsilon_n)$, for a spin. Then the probability of finding the spin in the local energy level j is written as

$$P_j = \exp(-\varepsilon_j/kT) \bigg/ \left(\sum_i \exp(-\varepsilon_i/kT)\right) \tag{1}$$

where k and T denote respectively the Boltzmann constant and temperature. If a random number R in the range $0 < R < 1$ comes into the region (Suzuki *et al* 1977, Miyashita 1982)

$$\sum_{j=1}^{m-1} P_j < R < \sum_{j=1}^{m} P_j \tag{2}$$

the spin is in the level m (see figure 1). When the distribution of the energy levels is

0022-3719/86/142539 + 08 $02.50

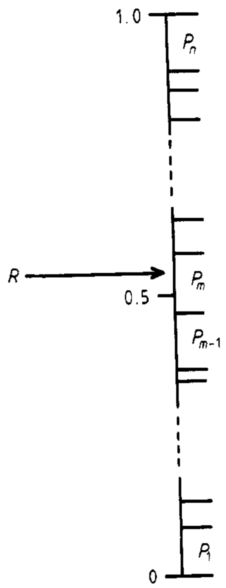

Figure 1. The Monte Carlo judgment for a spin with n local-energy levels. R denotes a random number.

continuous, the spin state m is determined by the following equation:

$$R = \int_1^m \mathrm{d}j\, P_j = F(m). \tag{3}$$

Thus, the state m is given by $m = F^{-1}(R)$, where F^{-1} denotes the inverse function of F.

The Hamiltonian that we consider as an example is

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} \boldsymbol{S}_i \cdot \boldsymbol{S}_j \tag{4}$$

where J (>0) denotes the exchange interaction between nearest-neighbour (NN) spins $\boldsymbol{S}_i$ and $\boldsymbol{S}_j$ and hence the summation runs over the NN pairs. Let us introduce the local-field vector at the ith spin through

$$\boldsymbol{H}_i = J \sum_{\rho} \boldsymbol{S}_{i+\rho} \tag{5}$$

where ρ denotes the vector directed to a nearest neighbour. Then the local Hamiltonian associated with $\boldsymbol{S}_i$ is written as

$$\mathcal{H}_l = -J\boldsymbol{S}_i \cdot \boldsymbol{H}_i = -JH\cos\theta \tag{6}$$

where $|\boldsymbol{S}_i| = 1$ and $|\boldsymbol{H}_i| = H$.

The probability of finding the spin i in an element of solid angle $\mathrm{d}\omega = \sin\theta\, \mathrm{d}\theta\, \mathrm{d}\phi$ is written as

$$P(\theta, \phi) \sin\theta\, \mathrm{d}\theta \mathrm{d}\phi = C \exp(-\mathcal{H}_l/kT) \sin\theta\, \mathrm{d}\theta\, \mathrm{d}\phi \tag{7}$$

where C denotes the normalisation constant

$$1/C = \int_0^{2\pi} \mathrm{d}\phi \int_0^{\pi} \sin\theta\, \mathrm{d}\theta \exp(-\mathcal{H}_l/kT). \tag{8}$$

Thus, θ and ϕ are determined by the following equations:

$$R = \int_0^{2\pi} \mathrm{d}\phi' \int_0^{\theta} \sin\theta' \, \mathrm{d}\theta' P(\theta', \phi') \tag{9a}$$

$$R' = \phi/(2\pi) \tag{9b}$$

where R and R' are random numbers both between 0 and 1. Solving equation (9*a*), we obtain

$$\cos\theta = (1/HK) \log[\exp(HK)(1 - R) + R\exp(-HK)] \tag{10}$$

where $K = J/kT$. The relation between R and $\cos\theta$ is shown in figure 2 for several values

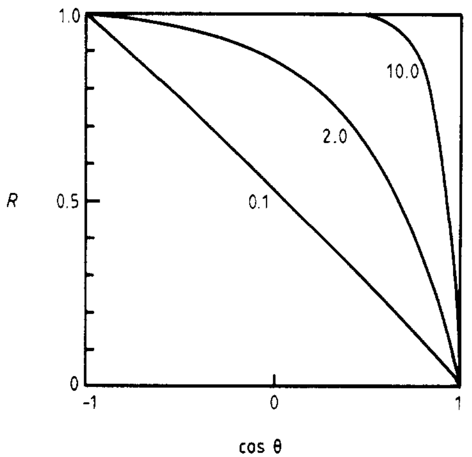

Figure 2. The relation between R and $\cos\theta$ for various values of HK given on the curves.

of HK. As seen from this figure, when the value of HK is small, the values of $\cos\theta$ are equally distributed with respect to the random number R. That is, the spins are randomly oriented at high temperatures. On the other hand, when the value of HK is large, the values of $\cos\theta$ are close to unity for most of the R-values. That is, the spins are almost parallel to each other at low temperatures.

Let us denote the components of $\boldsymbol{S}_i$ with respect to the crystal axes by (S_i^x, S_i^y, S_i^z) and the components of $\boldsymbol{S}_i$ with respect to the coordinate fixed to $\boldsymbol{H}_i$ by $(S_i^\xi, S_i^\eta, S_i^\zeta)$. Then we have

$$\begin{pmatrix} S_i^\xi \\ S_i^\eta \\ S_i^\zeta \end{pmatrix} = M(\Phi, \Theta, \Psi) \begin{pmatrix} S_i^x \\ S_i^y \\ S_i^z \end{pmatrix} \tag{11}$$

where $M(\Phi, \Theta, \Psi)$ denotes the usual rotation matrix associated with the Euler angles (Φ, Θ, Ψ). Using equations (9*a*) and (9*b*) we obtain $(S_i^\xi, S_i^\eta, S_i^\zeta)$. Finally, using equation (11), we obtain (S_i^x, S_i^y, S_i^z).

3. Results

We calculate the energy (per spin) using the following equation

$$u = (1/NJ)\langle\mathcal{H}\rangle \tag{12}$$

where N denotes the total number of spins and

$$\langle\mathcal{H}\rangle = \frac{1}{t-\tau}\int_{\tau}^{t} \mathrm{d}t'\, \mathcal{H}(t'). \tag{13}$$

Here t and τ have the usual meanings. In our calculation, we adopted the values $\tau =$ 4000 MC steps/spin and $t = 8000$ MC steps/spin. The specific heat and the susceptibility are defined by

$$c = K^2[\langle(\mathcal{H}/J)^2\rangle - \langle\mathcal{H}/J\rangle^2]/N \tag{14}$$

and

$$\chi = K[\langle(\sum_i S_i^z)^2\rangle - \langle\sum_i S_i^z\rangle^2]/N. \tag{15}$$

We note that the present MC method can be applied to the spin system with any anisotropic near-neighbour interactions

$$\mathcal{H} = -J\sum_{\langle i,j\rangle}(aS_i^xS_j^x + bS_i^yS_j^y + c'S_i^zS_j^z). \tag{16}$$

We performed the MC calculations for the following three cases: (i) the continuous-spin Ising model where $a = b = 0$ and $c' = 1$; (ii) the XY model where $a = b = 1$ and $c' =$ 0; (iii) the Heisenberg model where $a = b = c' = 1$.

Firstly, we show our MC computation results for the continuous-spin Ising model (Domb 1979, Binder 1976, Baker and Kincaid 1981), in which the random number R' of equation (9b) is not needed. The energy, specific heat, spin average and susceptibility for a two-dimensional continuous-spin Ising model are shown in figures 3–6 as functions of temperature. Here we assumed the square lattice with $N = 24^2$ spins and that the temperature was lowered gradually. The critical temperature is $T_c \cong 0.95J/k$. We note that the spin average

$$\bar{s} = \sum_i \langle S_i^z\rangle/N$$

completely vanishes above the critical temperature because we use the so-called long-time average (see equation (13)). For the three-dimensional continuous-spin Ising model, we show only the specific heat and the susceptibility (figures 7 and 8). We selected the simple cubic (SC) lattice with $N = 12^3$ spins. It is found that the critical temperature for this lattice is $T_c \cong 1.6J/k$. A high-temperature series calculation (Camp and Van Dyke 1975) predicts $T_c = 1.6639J/k$. On the other hand, the Metropolis MC value is $T_c = 1.748J/k$ (Binder and Rauch 1969). The continuous-spin Ising model for the face-centred cubic lattice has also been investigated by use of a high-temperature series expansion theory (Camp and Van Dyke 1975). This theory predicts $T_c =$ $3.5073J/k$. On the other hand, our MC value is $T_c \cong 3.45J/k$.

In figure 9, we show the specific heat of the XY model for the SC lattice. The deduced critical temperature is $T_c \cong 1.55J/k$. This value is close to the previous MC

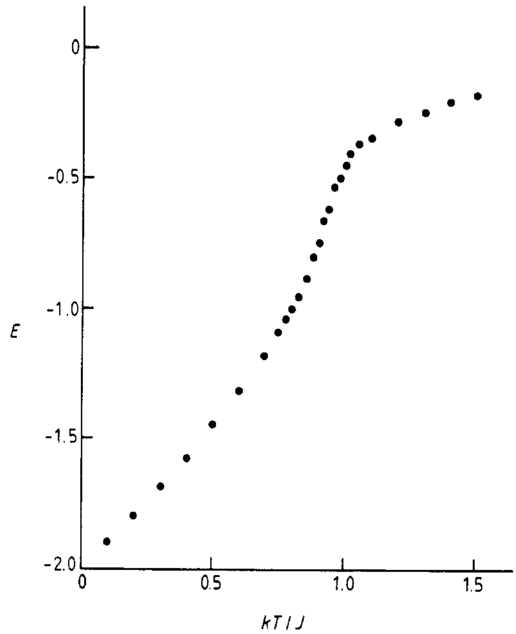

Figure 3. The energy of the two-dimensional continuous-spin Ising model.

value (Kawabata and Binder 1978). Finally, we show the specific heat of the Heisenberg model for the SC lattice in figure 10. We find that the critical temperature for the Heisenberg model is $T_c \cong 1.45J/k$. A high-temperature series expansion theory (Ritchie and Fisher 1972, Wood and Rushbrooke 1966) predicts $T_c = 1.445J/k$. On

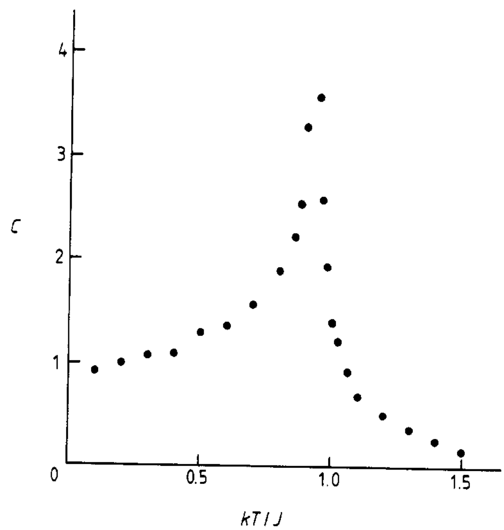

Figure 4. The specific heat of the two-dimensional continuous-spin Ising model.

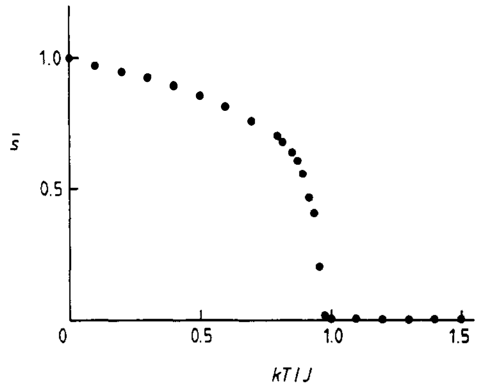

Figure 5. The spin average, $\bar{s}$, of the two-dimensional continuous-spin Ising model.

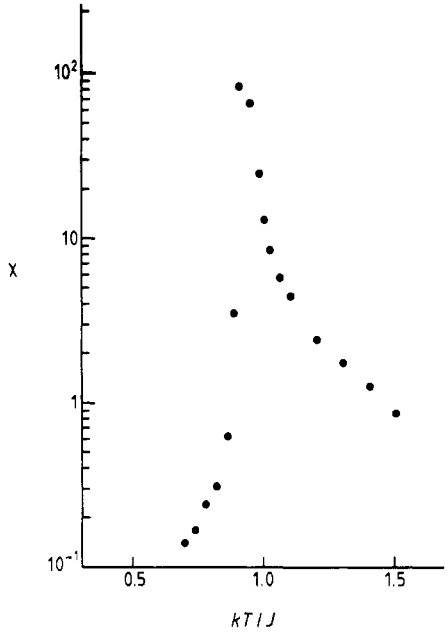

Figure 6. The susceptibility of the two-dimensional continuous-spin Ising model.

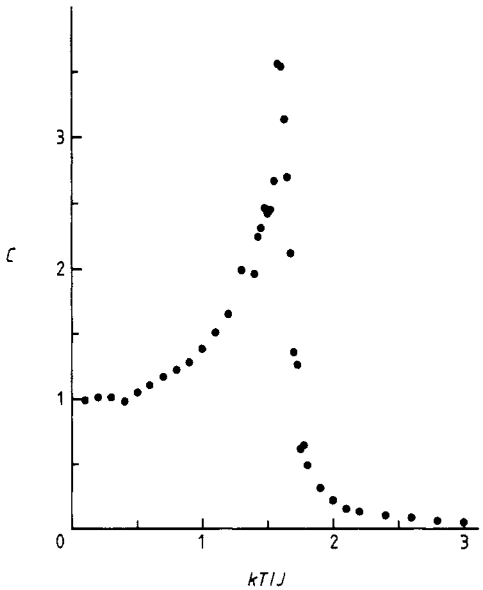

Figure 7. The specific heat of the three-dimensional continuous-spin Ising model.

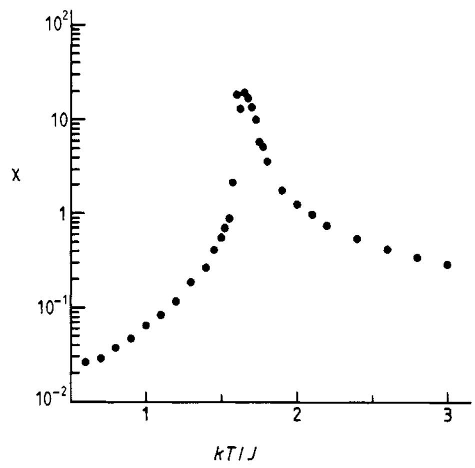

Figure 8. The susceptibility of the three-dimensional continuous-spin Ising model.

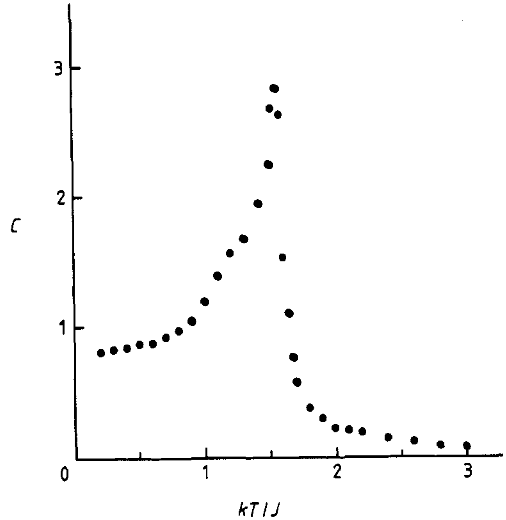

Figure 9. The specific heat of the three-dimensional *XY* model.

the other hand, the Metropolis self-consistent MC simulations (Müller-Krumbhaar and Binder 1972) also yield $T_c = 1.445J/k$.

4. Summary

We have reported in this paper on our recent MC calculations based on the 'heat bath' algorithms for various classical spin models. We find that our results are at least qualitatively in agreement with the previous results. We are hopeful that the present method may be utilised for various classical spin systems including spin glasses.

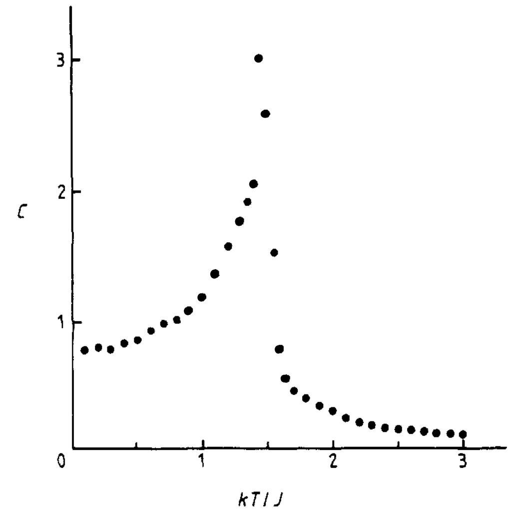

Figure 10. The specific heat of the three-dimensional Heisenberg model.

Acknowledgments

The authors would like to thank Professor M Suzuki and Dr S Miyashita of Tokyo University for valuable discussions. The authors also wish to thank Professor C Kawabata of Okayama University for letting them know of his previous work.

References

Baker G A Jr and Kincaid J M 1981 *J. Stat. Phys.* **24** 469
Binder K 1984 *Applications of the Monte Carlo Methods in Statistical Physics* (Berlin: Springer) p 1
—— 1976 *Phase Transitions and Critical Phenomena* vol 5b (London: Academic) p 29
Binder K and Rauch H 1969 *Z. Phys.* **219** 210
Camp W J and Van Dyke J P 1975 *Phys. Rev.* B **11** 2579
Domb C 1974 *Phase Transitions and Critical Phenomena* vol 3 (London: Academic) p 357
Fernandez J F and Streit T S J 1982 *Phys. Rev.* B **25** 6910
Källe C and Winkelman V 1982 *J. Stat. Phys.* **28** 639
Kawabata C and Binder K 1978 *Ann. Israel Phys. Soc.* **2** 988
Miyashita S 1980 *Prog. Theor. Phys.* **63** 797
Müller-Krumbhaar H and Binder K 1972 *Z. Phys.* **254** 269
Rebbi C 1984 *Applications of the Monte Carlo Methods in Statistical Physics* (Berlin: Springer) p 217
Ritchie D S and Fisher M E 1972 *Phys. Rev.* B **5** 2668
Suzuki M, Miyashita S and Kuroda A 1977 *Prog. Theor. Phys.* **58** 701
Teitel S and Jayaprakash C 1983 *Phys. Rev.* B **27** 598
Wood P J and Rushbrooke G S 1966 *Phys. Rev. Lett.* **17** 307