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Monte Carlo study of the three-state Potts model with two- and three-body interactions

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Abstract. A phase diagram of the three-state Potts model on a triangular lattice with two- and three-body interactions is obtained by computer simulations. The interactions allow antiferromagnetic as well as ferromagnetic phases. The ferromagnetic transition changes from continuous to first order on varying the coupling constants. The antiferromagnetic transition and the transition along the ferro- and antiferromagnetic coexistence line are first order. The resulting phase diagram agrees with that obtained by the low temperature series by Enting and Wu.

1. Introduction

The Potts model (Potts 1952) of phase transitions has recently become of particular interest, largely due to the richness of its physical content and its relevance in real physical systems (Domany *et al* 1977). While a large body of exact and rigorous results are now known (for a recent review see Wu (1982)), a number of problems, particularly those associated with models with antiferromagnetic and multi-site interactions, still remain unresolved. In this paper we address one such problem, the three-state model on a triangular lattice with two- and three-site interactions.

The system describes a Potts model in which each site can be in one of three spin states, 1, 2 or 3. The spins interact with a Hamiltonian which takes the form

$$-\frac{\mathcal{H}}{T}=K\sum_{(ij)}\delta_{\sigma_i\sigma_j}+L\sum_{(ijk)}\delta_{\sigma_i\sigma_j}\delta_{\sigma_j\sigma_k}. \tag{1}$$

Here and subsequently the Boltzmann constant k_B is set to be unity. $\sigma_i = 1, 2, 3$ specifies the spin state at the ith site, the first summation is over all nearest neighbouring pairs i and j of a triangular lattice, and the second summation is over *all* elementary triangular faces surrounded by sites i, j and k. The two- and three-site coupling constants K and L can be either positive or negative. With appropriate combinations of the couplings, the system can exhibit either a ferromagnetic or an antiferromagnetic transition.

The model (1) was first investigated by Schick and Griffiths (1977) by means of the real-space renormalisation group. Their result indicated that both the ferro- and antiferromagnetic transitions are continuous, and that the two transition lines meet at a bicritical point in the parameter space. More recently Enting and Wu (1982) studied this model by analysing the low-temperature series. While their analysis yielded a phase boundary, whose location is in general agreement with that determined

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from the renormalisation group, they also found different characters of the transitions. In particular, they found the transition of the antiferromagnetic model with pure two-site interactions and that along the (ferro- and antiferro-) coexistence line to be first order. Furthermore, their results suggest that the ferromagnetic transition changes from continuous to first order as the couplings are varied, thereby implying the existence of a tricritical point which is not revealed in the renormalisation group analysis. It is therefore pertinent to study this model using a different approach to clarify these points.

I have carried out a Monte Carlo simulation of the model (1). My main finding is a confirmation of the results implied by the low-temperature series analyses; I also obtained further data to pinpoint the location of the tricritical point.

2. Order Parameters

In figure 1 are shown the three distinct spin configurations which can occur around an elementary triangular face. They correspond to paramagnetic (P), ferromagnetic (F) and antiferromagnetic (AF) orderings. The energy per triangle for these configurations is $-TK/2$, $-TM/2$, and 0 respectively, where $M=3K+2L$. Therefore the ground state is P (without ordering) for $K>\{M, O\}$, F for $M>\{K, 0\}$ and AF for $0>\{M, K\}$. Our first task is to define an appropriate order parameter in the F and AF regions.

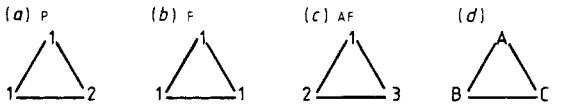

Figure 1. The three spin configurations of an elementary triangle typical of (*a*) the paramagnetic (P), (*b*) ferromagnetic (F) and (*c*) the antiferromagnetic (AF) states. (*d*) represents the sublattice structure in the AF state.

Let N_α, $\alpha=1, 2, 3$, denote the number of spins in the state $\sigma_i=\alpha$, with $\Sigma_{\alpha=1}^{3} N_\alpha = N$ being the total number of sites. Then the appropriate order parameter to take in the $N\to\infty$ limit of a ferromagnetic system is (Straley and Fisher 1973) $\hat{\phi}_F=\frac{3}{2}(\langle N_1/N\rangle-\frac{1}{3})$, where $\langle\,\rangle$ denotes the thermal average. However, since Monte Carlo simulations are done on finite lattices, and for all finite systems after a sufficiently long simulation $\hat{\phi}_F$ vanishes identically due to the symmetry of the Hamiltonian (1), $\hat{\phi}_F$ is not a good order parameter to use in practice. Instead, we take the quantity

$$m_F=\left\langle \tfrac{3}{2}\sum_{\alpha=1}^{3}(N_\alpha/N-\tfrac{1}{3})^2\right\rangle^{1/2} \tag{2}$$

as the ferromangetic order parameter. Clearly, $0\leqslant m_F\leqslant 1$, with $m_F=1$ denoting a complete ordering. We then define the susceptibility as

$$\chi_F=Nm_F^2/T, \qquad T>T_c, \tag{3}$$

as dictated by the fluctuation formula. Binder (1981) has defined the parallel and perpendicular susceptibilities, χ_1 and χ_2, as

$$\chi_1=\frac{1}{NT}(\langle N_1^2\rangle-\langle N_1\rangle^2), \qquad \chi_2=\frac{1}{2NT}[(\langle N_2^2\rangle-\langle N_2\rangle^2)+(\langle N_3^2\rangle-\langle N_3\rangle^2)].$$

In the paramagnetic phase ($T > T_c$) where $\langle N_\alpha \rangle = \frac{1}{3}N$, the system becomes isotropic and our susceptibility χ_F is essentially equivalent to χ_1 and χ_2:

$$\chi_F = \tfrac{9}{2}\chi_1 = \tfrac{9}{2}\chi_2.$$

It is expected that $m_F \sim O(1/\sqrt{N})$ and $\chi_F \sim O(1)$ in the paramagnetic phase.

When the system orders antiferromagnetically, the three sublattices A, B, C of the triangular lattice (cf figure 1(*d*)) are each occupied by a different spin state. Let N_α^x, $x = A, B, C$, denote the number of spins of state α in the sublattice x; then we define analogous to (2) the following (antiferromagnetic) order parameter:

$$m_{AF} = \left\langle \frac{3}{2} \sum_{\alpha \neq \beta \neq \gamma} \sum \sum \left(\frac{N_\alpha^A + N_\beta^B + N_\gamma^C}{N} - \frac{1}{3} \right)^2 \right\rangle^{1/2}. \tag{4}$$

When the system is in the AF state where most of the A sublattice sites are occupied by the spin species $\alpha = 1$, B by $\beta = 2$, and C by $\gamma = 3$, m_{AF} is approximately

$$m_{AF} \sim \frac{3}{2}\left\langle \left(\frac{N_1^A + N_2^B + N_3^C}{N} \right) - \frac{1}{3} \right)^2 \Big\rangle^{1/2} \sim \frac{3}{2}\left\langle \frac{N_1^A + N_2^B + N_3^C}{N} - \frac{1}{3} \right\rangle, \tag{5}$$

which is of O(1). In the P phase m_{AF} represents the antiferromagnetic fluctuation and becomes of $O(1/\sqrt{N})$. The assignment of the phases and phase transition in the Monte Carlo simulation is done with the help of the order parameters m_F and m_{AF}, as well as the internal energy per spin reduced by the temperature

$$E = -\langle \mathcal{H} \rangle / NT. \tag{6}$$

3. Ferromagnetic transition

Monte Carlo simulations are done for systems with various sizes $N = 15^2$, 30^2, 60^2, 120^2, with periodic boundary conditions. 4000 to 16 000 Monte Carlo steps per sites (MCS) are executed. Usually the first 200 MCS are discarded to allow for equilibrium. Due to the critical slowing down near the critical point, 1000 to 2000 MCS are necessary to reach equilibrium for some initial configurations. Especially near the tricritical point 2000 to 4000 MCS are used to equilibrate the system. In order to find the phase boundaries the coupling constants K and M are scanned along line l_1 ($L = 0$, $K > 0$), l_2 ($L > 0$, $K = 0$), l_3 ($M = -K > 0$), l_4 ($M = -0.6\,K > 0$), l_5 ($M = -0.2\,K > 0$), l_6 ($M = -0.1\,K > 0$), l_7 ($M = 0$, $K < 0$), l_8 ($M = K < 0$), l_9 ($L = 0$, $K < 0$), which are shown in the KM phase space in figure 2.

The line l_1 corresponds to the system with the ferromagnetic two-body interaction where the phase transition is known to be second order (Baxter 1973). The exact values of the transition coupling K_c (Kim and Joseph 1974) and of the internal energy E_c (Baxter *et al* 1978) are known: $K_c = \ln(2 \cos \pi/9) = 0.6309\ldots$, $E_c = 1.43908\ldots$. In figure 3(*a*) temperature (K) dependence of m_F and E obtained by Monte Carlo simulations is shown. At low temperatures (large values of K; $K > 0.63$), m_F's for various system sizes show no size dependence. At high temperatures ($K < 0.63$) m_F reveals clear size dependence, and the long-range ferromagnetic order vanishes in the thermodynamic limit. From this change in size dependence of m_F one may conclude that the transition takes place at $K = 0.630 \pm 0.002$, which agrees quite well with the exact value $K_c = 0.6309\ldots$. By fitting the magnetisation curve m_F to the scaling form $m_f \propto (1 - K_c/K)^\beta$ as is shown in figure 3(*a*), the magnetic critical exponent

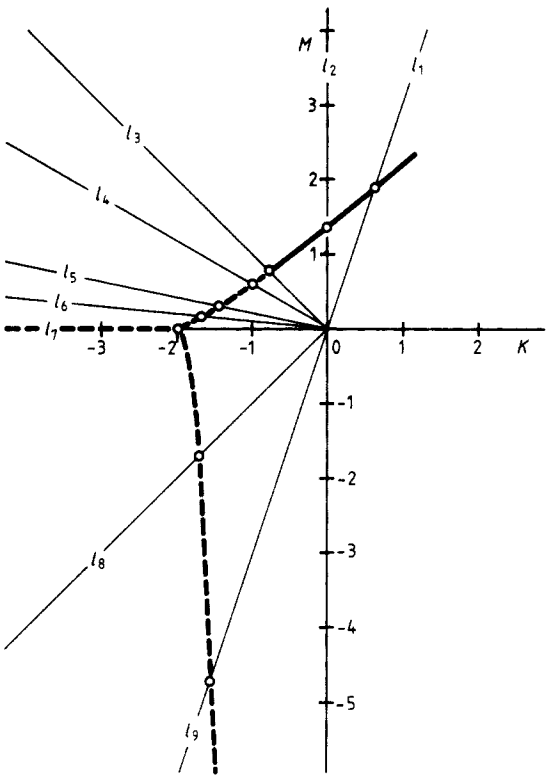

Figure 2. Phase diagram in KM space. Monte Carlo simulations are done along the line $l_1 \sim l_9$, and the obtained transition points are marked by circles. The full line represents the second-order transition, and the broken lines the first-order transition. The multicritical point is expected around $K \sim -0.77$.

$\beta = 0.10 \pm 0.01$ is obtained. As for the energy E, the size dependence appears only near the transition point for smaller systems ($N = 15^2, 30^2$), and the thermodynamic limit seems to be attained for larger systems ($N = 60^2, 120^2$). The critical value E_c of the energy obtained by Monte Carlo simulation agrees quite well with the exact value. By fitting E of the larger systems to the scaling forms, $E - E_c \propto (1 - K_c/K)^{1-\alpha'}$ for $K > K_c$ and $E_c - E \propto (K_c/K - 1)^{1-\alpha}$ for $K < K_c$, one obtains the critical exponents $\alpha' = 0.31 \pm 0.01$ and $\alpha = 0.35 \pm 0.03$. The high-temperature susceptibility, $\chi_F T = N m_F^2$, shown in figure 3(b), is almost independent of the size for $K < 0.62$ or $K_c/K - 1 \geq 0.05$. The fitting to the scaling form $\chi_F T \propto (K_c/K - 1)^{-\gamma}$ yields the value $\gamma = 1.3 \pm 0.2$. From figure 3(b) one finds the saturation of χ_F near the transition point. By assuming that χ_F's have already reached saturation values at $K = 0.63$ and further assuming a finite size scaling $\chi_F T \propto N^{\gamma/d\nu}$ for these saturation values, one obtains the exponent $\gamma/d\nu = 0.82$, or the exponent of the correlation length $\nu = 0.77$ by using $\gamma = 1.27$ and dimensionality $d = 2$. The resulting critical exponents are tabulated in table 1. They are consistent with those obtained by the previous Monte-Carlo simulations (Binder 1981). Monte Carlo renormalisation group (Rebbi and Swendsen 1980), or phenomenological renormalisation group theory (Nightingale and Blöte 1980) of the three-state Potts model on the square lattice, and agree well with the conjectured values (Enting 1975); $\alpha = \alpha' = \frac{1}{3}$, $\beta = \frac{1}{9}$, $\gamma = \frac{13}{9}$ and $\nu = \frac{5}{6}$.

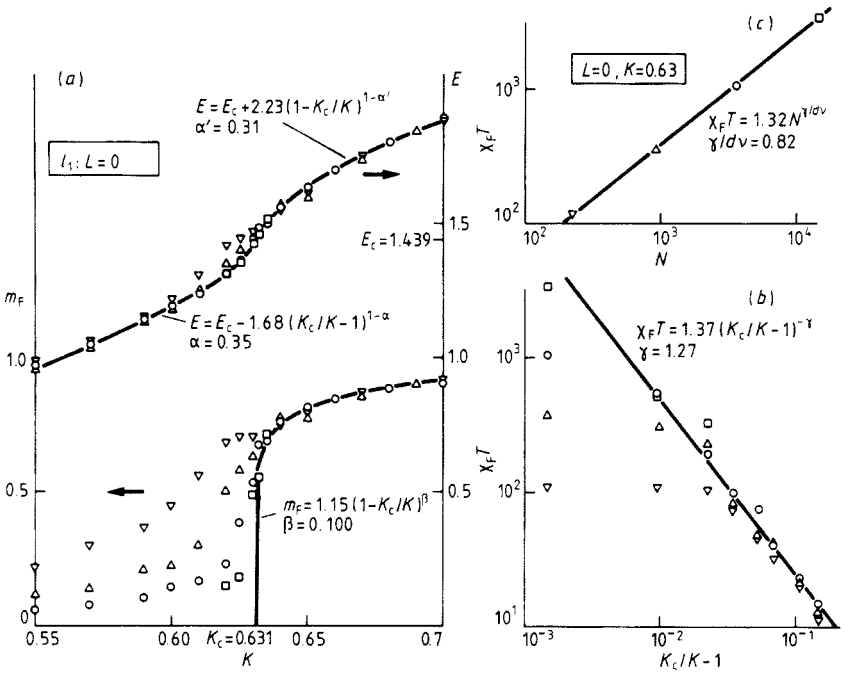

Figure 3. The simulation result with a pure two-body interaction (l_1): $L = 0$, $K > 0$ for various system sizes, N. ▽, $N = 15^2$; △, $N = 30^2$; ○, $N = 60^2$; □, $N = 120^2$. (*a*) The ferromagnetic order parameter m_F and the reduced energy E. The critical point and the fits to the scaling behaviour are also given. (*b*) The ferromagnetic susceptibility at high temperatures. (*c*) The saturation values of the ferromagnetic susceptibility at $K = 0.63$ are plotted as a function of the system size. The critical exponent ν is obtained to be 0.77.

Table 1. The Monte Carlo estimates of the second-order ferromagnetic transition temperatures and energies. Critical exponents are also estimated. The number in parentheses describes the uncertainty of the last digit.

	Transition	E_c	α	α'	β	γ	ν
$l_1: L = 0$	$K_c = 0.6309\ldots$	1.43094	0.35 (3)	0.31 (1)	0.10 (1)	1.3 (2)	0.8 (1)
$l_2: K = 0$	$M_c = 1.363$ (2)	0.86 (2)	0.40 (5)	0.42 (3)	0.11 (2)	1.2 (1)	—

For the case with pure three-body interaction (along l_2) the transition seems to be still continuous as is shown in figure 4(*a*). By fitting to the scaling form of the magnetisation and energy, we obtain the critical temperature $M_c = 1.363 \pm 0.002$ and the critical value of the energy $E_c = 0.86 \pm 0.02$. Critical exponents are obtained as $\alpha = 0.40 \pm 0.05$, $\alpha' = 0.42 \pm 0.03$, $\beta = 0.11 \pm 0.02$, $\gamma = 1.2 \pm 0.1$. The values of β and γ agree well with the conjecture values and represent the universality of the critical phenomena. The deviation of α and α' from the conjecture values may be due to the crossover to the first-order transition. The series expansion (Enting and Wu 1982) also reveals rather a large value $\alpha' \sim 0.65$.

Along the line l_3 ($M = -K > 0$) it is rather difficult to decide whether the transition is continuous or not. For very small systems ($N = 15^2, 30^2$) fluctuations are too large

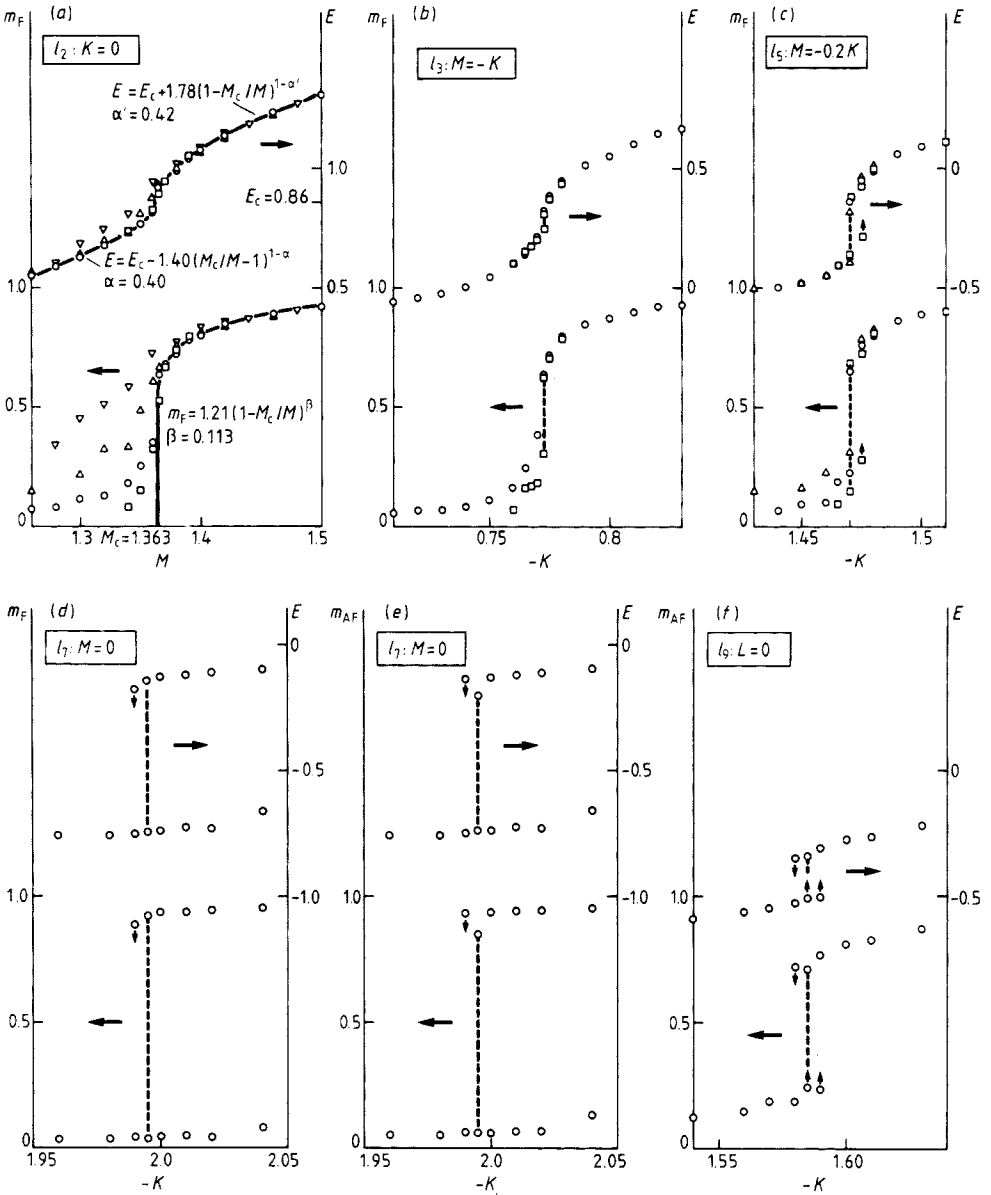

Figure 4. The energy E and the ferromagnetic (*a–d*) or the antiferromagnetic (*e*, *f*) order parameters along the lines (*a*) $l_2: K = 0$, (*b*) $l_3: M = -K$, (*c*) $l_5: M = -0.2K$, (*d*) and (*e*) $l_7: M = 0$ and (*f*) $l_9: L = 0$. Dotted lines represent the first-order phase transition, and the data points whith arrows indicate the (semi-) metastable states, which finally relax in the arrowed direction to the true stable state. ▽, $N = 15^2$; △, $N = 30^2$; ○, $N = 60^2$; □, $N = 120^2$.

to find the transition itself. For the system with size $N = 60^2$ we find no discontinuity in energy or magnetisation, whereas for the largest system, $N = 120^2$, tiny discontinuities in energy and in magnetisation are found, as is shown in figure 4(*b*).

The difference in behaviour may be attributed to the finite size effect, since in the small system the size masks the large but finite correlation length at the first-order transition point. We therefore conclude that along l_3 the system performs a weak first-order phase transition.

Along the lines $l_4 \sim l_7$ one finds rather large discontinuities in the energy and magnetisation, indicating first-order transitions. At the transition point, the ferromagnetic state obtained by heating the ferromagnetic initial state coexists with the paramagnetic state obtained by cooling the paramagnetic initial configuration, as are shown in figure 4(*c*) for l_5 and figure 4(*d*) for l_7. For l_7 ($M = 0$) a metastable paramagnetic state persists in low-temperature (large $-K$) regions, but for other cases, $l_4 \sim l_6$, the metastable state has relatively short lifetime and relaxes to the true equilibrium state as indicated by the arrows in figure 4. The first-order ferromagnetic transition points and the associated discontinuities in the energy and magnetisations are summarised in table 2. We expect a tricritical point near the line l_3 and $M \sim -K \sim 0.77$. The precise determination of the tricritical point and the values of the tricritical exponents, however, is very difficult from our restricted number of data points. Probably one has to use a Monte Carlo renormalisation group method to determine the location of the tricritical point, as has been done by Landau and Swendson (1981) for the Blume–Capel model. This is beyond the scope of the present paper.

Table 2. The estimates of the first-order ferromagnetic transition temperature, and discontinuities in energy and the ferromagnetic order parameter.

	K_c	ΔE	Δm_F
l_3: $M = -K$	−0.773	0.07	0.62
l_4: $M = -0.6\,K$	−0.1005	0.10	0.56
l_5: $M = -0.2\,K$	−1.470	0.26	0.67
l_6: $M = -0.1\,K$	−1.685	0.39	0.80
l_7: $M = 0$	−1.995	0.60	0.92

4. Antiferromagnetic transition

For $M \leqslant 0$ the antiferromagnetic structure, figure 1(*c*), is the ground state. We have performed Monte Carlo simulations with antiferromagnetic initial conditions, and found first-order antiferromagnetic transitions along the lines $l_7 \sim l_9$. Figure 4(*e*)

Table 3. The estimates of the first-order antiferromagnetic transition temperatures and the associated discontinuities in energy and the antiferromagnetic order parameter.

	K_c	ΔE	Δm_{AF}
l_7: $M = 0$	−1.995	0.54	0.85
l_8: $M = K$	−1.705	0.27	0.78
l_9: $L = 0$	−1.585	0.17	0.71

shows the change of the antiferromagnetic order parameter m_{AF} and the energy E along the line l_7 ($M=0$). By comparing figure 4(d) one finds F-AF coexistence regions at low temperatures $K<-1.995$. At the triple point $K_c=-1.995$ the P, F and AF phases coexist.

For the case with pure two-body antiferromagnetic interaction along the line l_9, the antiferromagnetic order parameter m_{AF} and the energy E are shown in figure 4(f). The transition temperature $K_c\sim-1.585$ and the energy discontinuity $\Delta E=0.17$ agree well with the values of the previous simulation by Grest (1981). The results of the antiferromagnetic transition temperatures and associated discontinuities in the energy and the antiferromagnetic order parameter are tabulated in table 3.

5. Summary

In conclusion, the Monte Carlo results are summarised in a phase diagram shown in figure 2. The ferromagnetic phase transisition in the positive M region changes from continuous to first order on varying the coupling constants. The antiferromagnetic phase transition in the negative M region and the transition along the ferro- and antiferromagnetic coexistence line at $M=0$ are first order. The obtained phase diagram agrees quantitatively with that obtained by the low-temperature expansion by Enting and Wu, except the position of the tricritical point which has large uncertainty anyhow. In order to determine the tricritical point, the real space renormalisation group method including the possibility of vacancy (for example Nienhuis *et al* 1979) may be applicable.

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