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Tricritical relaxation of the hard squares model with attractive next-nearest-neighbour interactions

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Abstract. The tricritical relaxation of the hard squares model with attractive next-nearest-neighbour interactions is studied. The dynamic exponent z_t of the model at its exactly known tricritical point is determined using the dynamic Monte Carlo renormalisation group method. The value of z_t is found to be 2.18 ± 0.11.

1. Introduction

The dynamic properties of kinetic Ising models have been extensively investigated in the past by a variety of analytic and computational methods. In particular, the dynamic Monte Carlo renormalisation group (DMCRG) method has provided accurate and systematically improvable estimates of the dynamic exponent z (Kalle 1984, Williams 1985 and references therein). While the dynamic critical properties of kinetic Ising models have been studied extensively, very few studies exist of the dynamic properties of tricritical models. In these models, the dynamic tricritical exponent z_t (dynamic exponent at the tricritical point) is also of interest in addition to the dynamic critical exponent z_c. The simplest tricritical models with well understood static properties occur in the universality class of (annealed) dilute Ising models. Well known examples are the Blume-Capel or the more general Blume-Emery-Griffiths (BEG) model and the Ising metamagnet (see e.g. Landau and Swendsen 1981). We note that the critical exponent z_c in the dynamic version of these models corresponds to the dynamic exponent of the pure Ising model. In three dimensions a direct Monte Carlo analysis of the Ising metamagnet with Glauber kinetics gave $z_t = 2.00$ (Müller-Krumbhaar and Landau 1976). This result which agrees with the conventional theory was subsequently confirmed by ε expansions (near four dimensions) on a similar model to all orders in ε (Siggia and Nelson 1977). By comparison, z_c in three dimensions was determined to be 2.02 using ε expansions (Bausch *et al* 1981), while a DMCRG analysis gave $z_c = 1.965 \pm 0.010$ (Kalle 1984). Recently, Achiam (1985, 1986) and Weir and Kosterlitz (1986) studied the one-dimensional kinetic BEG model and obtained $z_c = z_t = 2.00$.

In this study we analyse the dynamic tricritical exponent of a two-dimensional model. We study the kinetic hard squares lattice gas model with attractive next-nearest-neighbour interactions. The tricritical point of this model is in the same universality class as that of a dilute Ising model, and its location is known exactly (Huse 1983 and references therein). We estimate z_t through the DMCRG method used in the sense of Tobochnik *et al* (1981). We find $z_t = 2.18 \pm 0.11$. This value disagrees with the above

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mentioned ε expansion result of $z_t = 2.00$ found to all orders in ε. We can also make a comparison with z_c. In two dimensions, z_c, which corresponds to the dynamic critical exponent of the Glauber-Ising model, has been extensively studied in the past using a variety of methods. Two recent DMCRG analyses gave $z_c = 2.13 \pm 0.03$ (Williams 1985) and $z_c = 2.14 \pm 0.02$ (Kalle 1984). We note that our result for z_t is rather close to these values, considering the statistical accuracy of our calculation. This behaviour seems interesting in view of the rather different static exponents for the Ising-type critical and tricritical points (Nienhuis 1982). Clearly, a more accurate evaluation of z_t is necessary to be able to make a better comparison of z_c and z_t.

We present the model in § 2 with the method and calculations explained in § 3. Results are discussed in § 4.

2. The model

The Hamiltonian of the model is defined on the square lattice with an infinitely repulsive nearest-neighbour interaction (thus 'hard squares'). In addition there is an attractive interaction between next-nearest-neighbour pairs, and a chemical potential term. Thus, including the inverse temperature factor $(-\beta)$ the Hamiltonian is

$$-\beta\mathcal{H} = -J\sum_{\text{nn}} c_i c_j + K\sum_{\text{nnn}} c_i c_k + \mu\sum_i c_i \qquad J\to\infty,\ K>0 \tag{2.1}$$

where c_i is the lattice gas variable which can take on the values $c_i = 0$ or $c_i = 1$ and the sums Σ_{nn} and Σ_{nnn} extend over all nearest-neighbour and over all next-nearest-neighbour pairs, respectively. Transforming (2.1) into Ising-spin language with variables $\sigma_i = 2c_i - 1$ where $\sigma_i = \pm 1$ we arrive at the thermodynamically equivalent model:

$$-\beta\mathcal{H} = -\tfrac{1}{4}J\sum_{\text{nn}} \sigma_i\sigma_j + \tfrac{1}{4}K\sum_{\text{nnn}} \sigma_i\sigma_j + (-J + K + \tfrac{1}{2}\mu)\sum_i \sigma_i \qquad J\to\infty,\ K>0. \tag{2.2}$$

We note that the net effect of the J term in the limit $J\to\infty$ is to exclude all spin configurations with $(+,+)$ nearest-neighbour pairs from the partition sum. In the phase diagram, there is a paramagnetic phase in the region $K + \mu/2 \ll 0$, while in the region $K + \mu/2 \gg 0$ there is antiferromagnetic order with non-zero staggered magnetisation. The transition between the paramagnetic and antiferromagnetic phases is of the first order for large K giving rise to a first-order transition line in the phase diagram. For small K the transition is continuous and there is a critical line. The two transition lines are joined by a tricritical point. The location of the first-order line and the tricritical point have been exactly determined by Baxter (1980, 1982) in the context of a more general model. The tricritical point is located at $K = 1.6555\ldots$, $\mu = 3.2538\ldots$. Baxter's solution for the present model and the above features of the phase diagram were first pointed out by Huse (1982, 1983). The tricritical exponents of the model have turned out to be identical to those of a dilute Ising model, as suggested by the symmetry of the model (Huse 1982, 1983, Nienhuis 1982).

The dynamics of the model is the relaxational, non-conserved order parameter dynamics generated by the standard spin-flip Monte Carlo procedure (Binder 1976). A site on the lattice is chosen at random, the energy change which would result from flipping the spin on that site is calculated and the spin is flipped according to the probability $\min\{\exp(-\Delta E), 1\}$. Time is measured in Monte Carlo steps per spin (MCS). We note that there are two critical parameters at the tricritical point of our model as

is characteristic of a tricritical system (Riedel and Wegner 1972). These are the staggered magnetisation (order parameter) and the magnetisation (non-ordering parameter). This implies that in the dynamics there are two independent modes which exhibit critical slowing down at the tricritical point. However, we expect that as in critical dynamics there will be a single relevant timescale at the tricritical point determined by the slowest relaxation mechanism in the system, and this timescale will govern the behaviour of the time correlation functions and hence the dynamic exponent.

3. Method and calculations

Several variants of the DMCRG method exist at present. The basic idea utilised by all formulations is the dynamic scaling which states that if the length scale of a system changes by a factor b upon renormalisation, then the timescale must change by a factor b^z. In the procedure introduced by Tobochnik *et al* (1981) two systems with sizes L and bL are simulated by the Monte Carlo method. Renormalised systems are obtained from the configurations of the original lattices by using (typically) the majority-rule blocking, which reduces the size of the system by a factor of b. One then attempts to find two times, t and t', such that the time correlation functions evaluated on the smaller lattice after m blockings 'match' those evaluated on the larger lattice after $m+1$ blockings. According to dynamic scaling t and t' must be related as $t' = tb^z$. This then determines z.

In the version of the DMCRG developed by Katz *et al* (1982) the matching is applied in the long-time regime in which the time correlations are expected to have a simple exponential behaviour. This approach is known to be equivalent to a finite-size scaling analysis (Williams 1985).

A different formulation of the DMCRG was also developed by Jan *et al* (1983). In this procedure the matching is done in the short-time regime using the non-equilibrium averages of magnetisation.

In this study we have utilised the DMCRG in the sense of Tobochnik *et al* (1981). In our calculations we have used the same-site time correlation function Γ:

$$\Gamma(L, m; t) = (N^{(m)})^{-1}\left\langle \sum_i \sigma_i^{(m)}(0)\sigma_i^{(m)}(t) \right\rangle. \tag{3.1}$$

Here, L is the lattice size, m is the number of renormalisation transformations performed, $N^{(m)}$ is the number of block spins on the mth renormalised lattice and $\sigma_i^{(m)} = \pm 1$ are the block-spin variables. Since the simulations are performed at the tricritical point, successive renormalisation transformations are expected to lead to a fixed point, and for sufficiently large m we expect the matching condition

$$\Gamma(L, m; t) = \Gamma(bL, m+1; tb^z). \tag{3.2}$$

To check the extent of the approach to the fixed point one can compare static quantities on the renormalised lattices, since these quantities are expected to match near the fixed point. For this reason we have also calculated the next-nearest-neighbour static correlation function C:

$$C(L, m) = (N^{(m)})^{-1}\left\langle \sum_{\text{nnn}} \sigma_i^{(m)}\sigma_k^{(m)} \right\rangle. \tag{3.3}$$

(The nearest-neighbour correlation function in our model is proportional to the magnetisation. Thus this quantity displays large fluctuations.)

We have performed our simulations on two initial lattices with sizes $L=54$ and $L=18$. Renormalised lattices have been obtained by applying the majority rule with 3×3 blocks (hence $b=3$ in our analysis) as shown in figure 1. We have employed periodic boundary conditions and random initial configurations. The averages have been performed by using 150 independent runs of 2×10^4 MCS for the 54×54 lattice and 180 independent runs of 1×10^4 MCS for the 18×18 lattice. Our error estimates are based on the spread of the data in these independent runs. The results for C are shown in table 1. We note that the static quantities $C(L, m)$ and $C(bL, m+1)$ are off by about three standard deviations for the 18×18 renormalised lattices, while they match well within one standard deviation for the 6×6 renormalised lattices. This indicates that while the effects of the irrelevant operators still exist after the first renormalisation, they are sufficiently reduced through the second renormalisation to give us a fixed point behaviour. 2×2 renormalised lattices have been excluded from our analysis because lattices of this size are not expected to encompass the range of interactions in the fixed-point Hamiltonian.

We now turn to the dynamic quantities. In table 2 we show results for $\Gamma(t)$ evaluated at time values which differ by a factor of nine on the two initial lattices. If there were perfect matching of Γ values this would give $z_t=2$ due to equation (3.2). Since there is not perfect matching, we use the values of Γ at intermediate time values for the

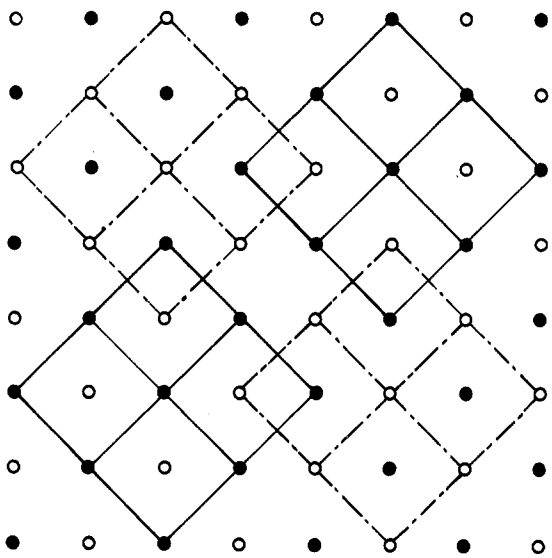

Figure 1. The block construction used in the RG transformation. Full and open circles represent the two sublattices of the initial model while the 3×3 blocks constructed with full and broken lines represent the two sublattices of the renormalised model.

Table 1. Results for $C(L, m)$, for $L=18$ and 54.

m	$C(54, m)$	m	$C(18, m)$
0	0.8014 ± 0.0021		
1	0.8203 ± 0.0019	0	0.8122 ± 0.0012
2	0.8508 ± 0.0024	1	0.8519 ± 0.0017

Table 2. Results for $\Gamma(L, m; t)$ and z_t, for $L = 54$ and 18.

t	m	$\Gamma(54, m; t)$	t	m	$\Gamma(18, m; t)$	z_t
99	0	0.6213 ± 0.0047	11			
	1	0.7293 ± 0.0029		0	0.7148 ± 0.0018	
	2	0.8542 ± 0.0021		1	0.8471 ± 0.0016	2.16 ± 0.08
198	0	0.6033 ± 0.0043	22			
	1	0.7059 ± 0.0034		0	0.6911 ± 0.0022	
	2	0.8272 ± 0.0027		1	0.8195 ± 0.0021	2.18 ± 0.10
297	0	0.5942 ± 0.0050	33			
	1	0.6963 ± 0.0040		0	0.6791 ± 0.0024	
	2	0.8120 ± 0.0034		1	0.8042 ± 0.0024	2.19 ± 0.14

initial 18×18 lattice and apply interpolation to obtain the times which would give perfect matching. This procedure has been carried out for three different time values ($t = 99$, 198 and 297) for the initial 54×54 lattice and resulted in the three estimates of z_t given in table 2. Since the static quantities match properly only for the 6×6 renormalised lattices, the z_t estimates have been included only for these lattices. The average of the three estimates given in table 2 results in the final average $z_t = 2.18 \pm 0.11$.

4. Conclusions

We have determined the dynamic tricritical exponent z_t of the hard squares model with attractive next-nearest-neighbour interactions. The tricritical point of this model is in the same universality class as the tricritical point of a dilute Ising model. We have used the DMCRG method to obtain the estimate $z_t = 2.18 \pm 0.11$. This value is in disagreement with the ϵ-expansion (around four dimensions) result $z_t = 2.00$ (Siggia and Nelson 1977). However we cannot strictly compare the two results, for although the result $z_t = 2.00$ was obtained to all orders in ϵ, there is clearly little reason to expect it to be valid for two dimensions. As we remarked in § 1, another aspect of our result is that our value for z_t appears to be rather close (in fact, equal within statistical accuracy) to the values found in previous studies for the corresponding (Ising) dynamic critical exponent z_c. While there seems no theoretical reason for the equality or even closeness of z_c and z_t, the same behaviour also occurs in the one- and three-dimensional cases, as can be seen from the results of previous studies stated in § 1. Nevertheless, for the two-dimensional case treated here a more accurate evaluation of z_t is necessary to draw a conclusion in this respect. Further work in our analysis is also necessary to ensure the convergence of our estimates. For this, one needs to perform further RG steps, which requires bigger initial lattices and consequently much longer computation times. An implementation of DMCRG, which uses short-time non-equilibrium averages as in the method of Jan *et al* (1983) might be computationally more efficient in this respect. Finally, we must point out that in our analysis we have not considered any small shift in the tricritical point arising from finite-size effects. Although in principle such a shift might prevent the renormalised systems from properly converging onto the tricritical fixed point, in view of the relatively large tricritical region in our model (the crossover exponent $\phi = 0.44$ (Nienhuis 1982)) we regard this behaviour as unlikely.

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