Non-equilibrium phase transitions in one-dimensional kinetic Ising models

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Abstract. A family of non-equilibrium kinetic Ising models, introduced earlier, evolving under the competing effect of spin flips at *zero temperature* and nearest-neighbour random spin exchanges, is further investigated. By increasing the range of spin exchanges and/or their strength the nature of the phase transition 'Ising-to-active' becomes of (dynamic) mean-field type and a first-order tricitical point is located at the Glauber ($\delta = 0$) limit. Corrections to the mean-field theory are evaluated up to sixth order in a cluster approximation and found to give good results concerning the phase boundary and the critical exponent β of the order parameter which is obtained as $\beta \simeq 1.0$.

1. Introduction

Kinetic Ising models were originally intended to study relaxational processes near equilibrium states [1,2]. Later combinations of Glauber and Kawasaki dynamics were used successfully in investigating questions about temperature-driven non-equilibrium phase transitions [3–5]. In a previous paper a class of general non-equilibrium kinetic Ising models (NEKIM) with combined spin-flip dynamics at $T = 0$ and spin-exchange dynamics at $T = \infty$ has been introduced [6], in which, for a range of parameters (other than temperature) of the model, a directed-percolation-like Ising-to-active phase transition takes place. The line of phase transitions have been found to belong to the same universality class as the phase transitions occurring in the cellular automaton models introduced and investigated by Grassberger *et al* [7, 8]. Numerical studies of other models showing similar types of phase transition have been reported recently [9, 10].

In this paper we consider a generalized form of NEKIM by allowing for exchanges of arbitrary range, R. The mean-field (MF) limit of NEKIM phase transitions is reached when $R \to \infty$ and/or the probability of the exchanges, p_{ex}, relative to the time scale of spin-flips approaches infinity. In a systematic generalized MF approach (GMF) [11–13], besides the lowest-order approximation (ordinary dynamic MF, $n = 1$) the second-order cluster equations ($n = 2$) could also be solved exactly. Numerical solutions have been obtained up to sixth order.

In this way we have found strong theoretical evidence for the conjecture, stemming from simulations [6], that the line of Ising-to-active second-order phase transition points ends at the Glauber limit ($\delta_c = 0$, δ being a parameter of the spin-flip transition rate of crucial importance here) with maximal exchange range and/or rate. It is shown here that this end point is of first order (tricritical point) and is described by plain MF theory. The relaxation

time is obtained as $\tau \propto 1/|\delta|$. GMF results show that with increasing n the critical point becomes of second order and moves towards negative values of δ of increasing absolute value. The coherent anomaly method [14, 15] has been used to extract the exponent β of the order parameter from the results of GMF calculations yielding $\beta = 1.0$.

2. The model

In NEKIM we have started with the general form of the Glauber [1] spin-flip transition rate in one dimension for spin s_i sitting at site i ($s_i = \pm 1$):

$$w_i = \Gamma/2(1 + \delta s_{i-1}s_{i+1})\left(1 - \tfrac{1}{2}\gamma s_i(s_{i-1} + s_{i+1})\right) \tag{1}$$

where $\gamma = \tanh 2J/kT$ (J denoting the coupling constant in the Ising Hamiltonian), Γ (denoted by $1/\Gamma$ in [6]) and δ are further parameters which can, in general, also depend on temperature. When $T = 0$ is taken then $\gamma = 1$ and (1) leads to two independent rates:

$$p_{RW} \equiv 2w_{\uparrow\downarrow\downarrow} = \Gamma(1 - \delta) \qquad p_{an} \equiv w_{\uparrow\downarrow\uparrow} = \Gamma(1 + \delta) \tag{2}$$

responsible for random walk and pairwise annihilation of kinks, respectively. Γ and δ are constants to be varied.

The other ingredient of NEKIM has been a spin-exchange transition rate of neighbouring spins (the Kawasaki [2] rate at $T = \infty$):

$$w_{ii+1} = \tfrac{1}{2}p_{ex}[1 - s_i s_{i+1}] \tag{3}$$

where p_{ex} is the probability of spin exchange. p_{RW}, p_{an} and p_{ex} have been chosen as normalized to unity, leading to the relation
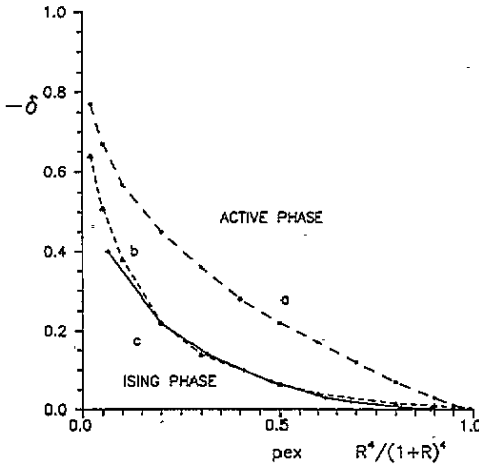
$$p_{ex} = 1 - 2\Gamma. \tag{4}$$

The spin-exchange process induces pairwise creation of kinks in the immediate neighbourhood of an existing kink: $k \to 3k$ with probability p_{ex}. From this process the ultimate development of an active phase can arise and in [6] we have made the conjecture, and found numerical evidence for it, that $p_{RW} > p_{an}$ (i.e. $\delta < 0$) is necessary for this to happen.

Now we generalize the original NEKIM model by allowing the range of the spin-exchange to vary. Namely, equation (3) is replaced by

$$w_{i,i+k} = \tfrac{1}{2}p_{ex}[1 - s_i s_{i+k}] \tag{5}$$

where i is a randomly chosen site and s_i is allowed to exchange with s_{i+k} with probability p_{ex}. Site k is again randomly chosen in the interval $1 \leqslant R$, R thus being the range of exchange. The spin-flip part of the model will be unchanged. We have carried out numerical studies with this generalized model in order to locate the lines of Ising-to-active phase transitions. Spin-flip and spin-exchange have been applied alternately at each time step, the spin-flip part has been applied using two-sublattice updating, while making l Monte Carlo attempts at random (l denotes the size of the chain) has been counted as one time-step of exchange updating. It is worth mentioning that, besides $k \to 3k$, the process $k \to 5k$ can also occur for $R \geqslant 3$, and the new kink pairs are not necessarily neighbours. The character of the phase transition line at $R > 1$ is similar to that for $R = 1$, except that the active phase extends, asymptotically, down to $\delta_c = 0$. This is illustrated in figure 1, where besides $R = 1$, the case $R = 3$ is also depicted: the critical value of $-\delta_c$ is shown as a function of p_{ex} (figure 1, curves a and b). Moreover, $-\delta_c$ as a function of R is also shown at constant $\Gamma = 0.35$. The abscissa has been suitably chosen to squeeze the whole (infinite) range of

Figure 1. Phase diagram of NEKIM for $\delta_c(R, p_{ex})$ is depicted for: a, $R = 1$; b, $R = 3$ as a function of p_{ex} (with $2\Gamma = 1 - p_{ex}$) and c, $\Gamma = 0.35$ ($p_{ex} = 0.3$) as a function of $(R/1 + R)^4$ (full curve). The phase boundaries have also been obtained by measuring $\rho(t)$, the density of kinks, starting from a random initial distribution and locating the phase transition points by $\rho(t) \propto t^{-\alpha}$ with $\alpha = 0.27 \pm 0.04$. Typically the number of lattice points has been $l = 2000$ with averaging over 500 independent runs.

R between 0 and 1 and for getting phase lines of comparable size (hence the power of 4 of $R/(1 + R)$ in the case of figure 1, curve (c)).

Besides the critical exponent α, used in identifying the phase transition points, also the other critical exponents characterizing the phase transition have been determined numerically around some typical points (far from the end points) of the phase transition lines for $R > 1$, with the same result as obtained in [6] for the case $R = 1$: the exponents agree, within errors, with those of Grassberger's automata [7, 8].

On the phase diagrams of figure 1 two non-typical regimes can be distinguished, namely:

(i) $p_{ex} \approx 0$ (figures 1, curves a and b). Here NEKIM's behaviour is getting close to that of the plain spin-flip model at $T = 0$: the steady state is everywhere Ising-like except for the limit-point $\delta = -1$, where $p_{an} = 0$ and the initial kink density is sustained. At this specific point the energy becomes conserved with a change in the form of the time dependence of correlations from exponential to stretched exponential [16]. This limit will not be discussed further here.

(ii) $p_{ex} \approx 1.0$ and/or $R \to \infty$ (figures 1, curves a–c). For $p_{ex} \to 1$, $R = 1$ we have concluded in [6] that $\delta_c \to -0$, though it has been difficult to get reliable numerical estimates for the critical exponents of the transition due to the long transients.

In (ii), after each step of spin-flip ordering, maximal mixing of the neighbourhood of each spin follows, suggesting that a mean-field type situation takes place. It is important that according to (4) $p_{ex} = 1$ is approached together with $\Gamma \to 0$ and thus $p_{ex}/\Gamma \to \infty$. (As Γ sets the time scale of the ordering process, its vanishing tendency enhances the effect of mixing). The same limit can be reached at fixed p_{ex} by increasing R to infinity (figure 1, curve (c)).

We have also checked the decrease of $-\delta_c$ with $1/R$ numerically at fixed $\Gamma = 0.35$, $p_{ex} = 0.3$ and found, over the decade of $R = 4$–40, that

$$-\delta_c \approx 2.0(1/R)^2 \tag{6}$$

reminiscent of a crossover-type behaviour of equilibrium and non-equilibrium phase transitions [17], here with crossover exponent $\frac{1}{2}$. It should be noted here, that to get closer to the expected $\delta_{cMF} = 0$, longer chains (we used l values up to 20 000) and longer runs (here up to $t = 5 \times 10^4$) would have been necessary. The former to ensure $l \gg R$ [18] and the latter to overcome the long transients present at the first few decades of time steps.

In what follows we will always refer to the MF limit in connection with $p_{ex} \rightarrow 1$ (i.e. $p_{ex}/\Gamma \rightarrow \infty$), for the sake of concreteness, but keep in mind that $R \rightarrow \infty$ can play the same role.

3. Mean-field theory and corrections to mean field

It is straightforward to find the MF equation for the spin-flip model alone (at $T = 0$). By denoting the average spin density by M we get, using (1)

$$dM/dt = -\delta\Gamma M(M^2 - 1). \tag{7}$$

The fixed-point solutions are $M^* = 1, -1, 0$ of which the first two are stable if $\delta > 0$, while the $M^* = 0$ solution is stable for $\delta < 0$, suggesting a (first-order) order–disorder-type phase transition at $\delta = 0$. That the $M^* = 0$ fixed-point is not an antiferromagnetic type can be shown by carrying out a two-sublattice MF analysis of the model [19]. First sublattice: odd lattice points with average magnetization M_1, second sublattice: even lattice points with average magnetization M_2. The total average magnetization $M = (M_1 + M_2)/2$ and the difference of the sublattice magnetizations $\Delta = (M_1 - M_2)/2$ obey the following MF equations:

$$dM/dt = -\delta\Gamma M(M^2 - 1 - \Delta^2) \tag{8}$$

$$d\Delta/dt = -2\Gamma\Delta + \delta\Gamma\Delta(M^2 - 1 - \Delta^2). \tag{9}$$

The solutions for fixed-point $\Delta^* \neq 0$ are: $M^* = 0$, $\Delta^{*2} = -1 - \frac{2}{\delta}$.

With values of δ restricted to $1 \geqslant \delta \geqslant -1$, the only possibility to ensure $\Delta^{*2} > 0$ at the same time is: $\delta = -1$, with $\Delta^{*2} = 1$. Thus we will suppose that the transition at $\delta_c = 0$ is of order–disorder type. A small fluctuation dM around one of the stable fixed-points decreases as $dM \propto e^{-t/\tau}$ with $\tau = 1/\Gamma|\delta|$. This relaxation time becomes infinite at the MF transition point. The corresponding critical slowing down in its vicinity explains the longer and longer transients observed during simulations.

Figure 2 serves to illustrate the MF result in comparison with results of simulation of NEKIM. The average density of kinks at $t = \infty$ is depicted versus δ. The MF approximation corresponds to figure 2, curve a, with a jump at $\delta_{cMF} = 0$. Figure 2, curve b, shows the
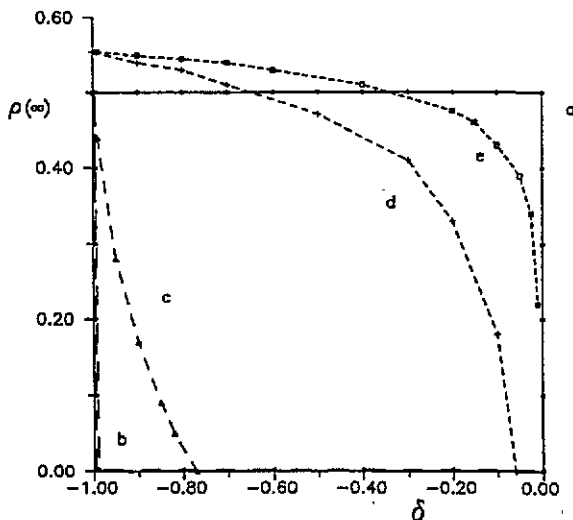

Figure 2. Kink density ρ in the steady state as a function of δ: a, result of first-order MF calculation with a jump at $\delta = 0$, reflecting the first-order nature of the transition; b, the same quantity for the pure spin-flip model: $\rho(\infty) = \rho(0)$ at $\delta = -1$, otherwise $\rho(\infty) = 0$. c, d, e: results of simulations of NEKIM, see the text.
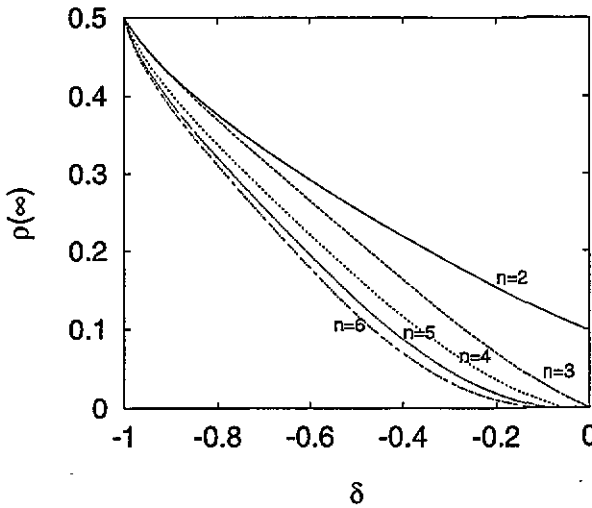
Figure 3. $\rho(\infty)$ as a function of δ as obtained from GMF for $n = 3, \ldots, 6$ in the case of $\Gamma = 0.35$

behaviour of the pure spin-flip model at $T = 0$: the steady state is everywhere Ising-like ($\rho(\infty) = 0$) except for $\delta = -1$. Figures 2, curves c–e are results of simulation of NEKIM at $p_{ex} = 0.02$, $p_{ex} = 0.9$ and $p_{ex} = 0.98$, respectively. By further decreasing (increasing) p_{ex}, the NEKIM curves get closer and closer to b (or a, respectively). Such behaviour is in accordance with our expectations: it supports the MF interpretation of the high-p_{ex} part of the phase diagram.

We have applied the generalized mean-field calculation method, or cluster approximation [11, 12] in the form applied for cellular automata [13] in order to go beyond the lowest-order approximation shown above.

Steady-state equations have been set up for block probabilities in $n = 2 \ldots$ 6th order. The system of GMF equations is solvable analytically also for $n = 2$.

The $n = 2$ approximation gives the density of kinks $\rho(\infty)$ as

$$\rho(\infty) = \frac{\frac{3}{4}p_{RW}^2 + p_{an} - p_{RW}p_{an} - \sqrt{\frac{1}{16}p_{RW}^4 + \frac{3}{2}p_{RW}^2 p_{an} - \frac{1}{2}p_{RW}^3 p_{an} + p_{an}^2 - 2p_{RW}p_{an}^2}}{2\left(\frac{1}{2}p_{RW}^2 - p_{RW}p_{an} + p_{an}^2\right)}$$

(10)

for $\delta < 0$. For $\delta > 0$, $\rho(\infty) = 0$, i.e. GMF still predicts a first-order transition for $\delta = 0$; the jump in $\rho(\infty)$ at $\delta = 0$, however, decreases monotonically with decreasing Γ, according to (10) and (2).

In order to get the $n > 2$ approximations, the set of GMF equations can only be solved numerically. We determined the solutions of the $n = 3, 4, 5, 6$ approximations for the kink density at (i) $\Gamma = 0.35$ (figure 3) and of the $n = 3, 4, 5$ approximations at (ii) $\Gamma = 0.05$ (figure 4). As we can see the transition curves became continuous, with negative values for δ_c^n (δ_c^n denotes the value of δ in the nth approximation for which the corresponding $\rho(\infty)$ becomes zero). Moreover, $|\delta_c^n|$ increases with growing n values. As increasing n corresponds to decreasing mixing, i.e. decreasing p_{ex}, the tendency shown by the above results is correct.

Figures 5(a) and 5(b) show a quantitative—though only tentative—comparison between the results of GMF and the simulated NEKIM phase diagrams. The obtained GMF data for δ_c^n corresponding to $n = 3, 4, \ldots, 6$ ($\Gamma = 0.35$) are depicted in figure 5(a) as a function of $1/(n - 3)$, together with results of simulations. The correspondence between n and p_{ex} has
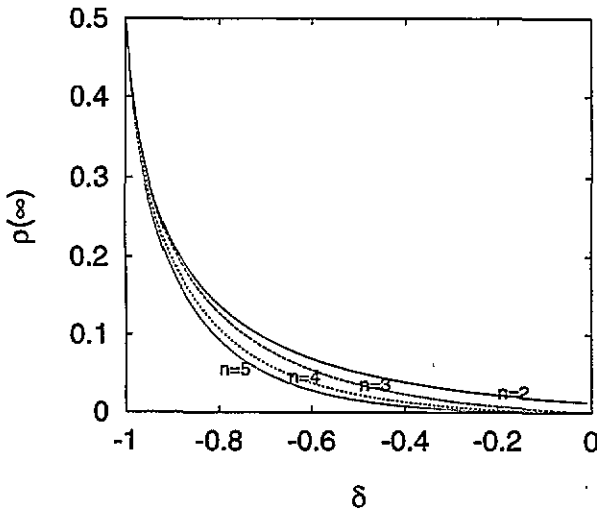
Figure 4. Kink density $\rho(\infty)$ obtained by GMF for $n = 3, 4, 5$ in the case of $\Gamma = 0.05$
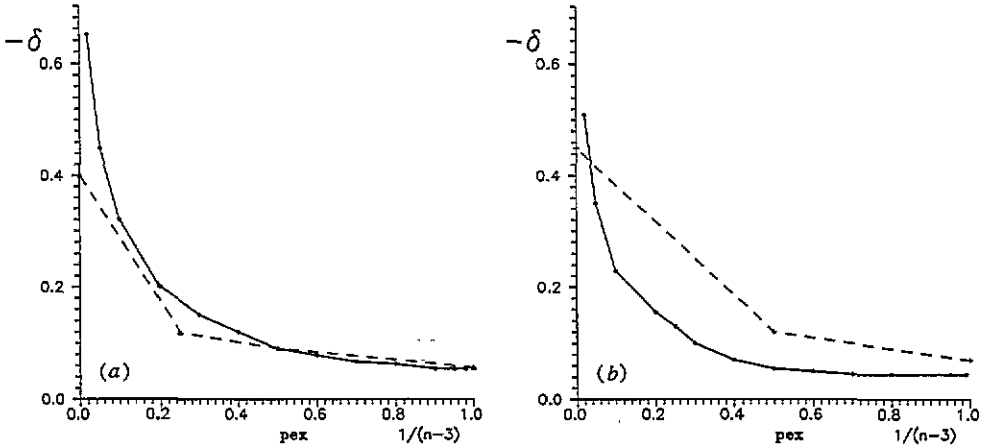

Figure 5. Comparison between results of simulation and GMF: GMF results for δ_c are plotted as a function of $1/(n - 3)$, while simulation results for δ_c are depicted as a function of p_{ex} at *constant* Γ, with $R = 3$ in the case of (*a*) $\Gamma = 0.35$ and (*b*) with $R = 1$ for $\Gamma = 0.05$.

been chosen as the simplest conceivable one (note that $\delta_c \neq 0$ is obtained first for $n = 4$). The simulated phase diagram has been obtained without requiring the fulfillment of (4), at constant $\Gamma = 0.35$. In this case the $\delta_c = 0$ limit, of course, is not reached and a purely second-order phase transition line can be compared with GMF results (for n values where it also predicts a second-order transition). Simulations for $R = 3$ have been found to lead to $|\delta_c|$ values low enough to fit GMF data. The (polynomial) extrapolation of GMF data to $n \to \infty$ (corresponding to $p_{ex} = 0$, i.e. plain spin-flip), also shown in figure 5, could have been expected to approach $\delta = -1$. That this is not the case can be ascribed to the circumstances that (i) GMF starts here from a first-order MF phase transition, (ii) which, upon increasing n, becomes second order and (iii) the point it should reach for $n \to \infty$ is again a first-order transition point, discussed shortly in section 2, with quite unusual (and not yet completely cleared up) properties.
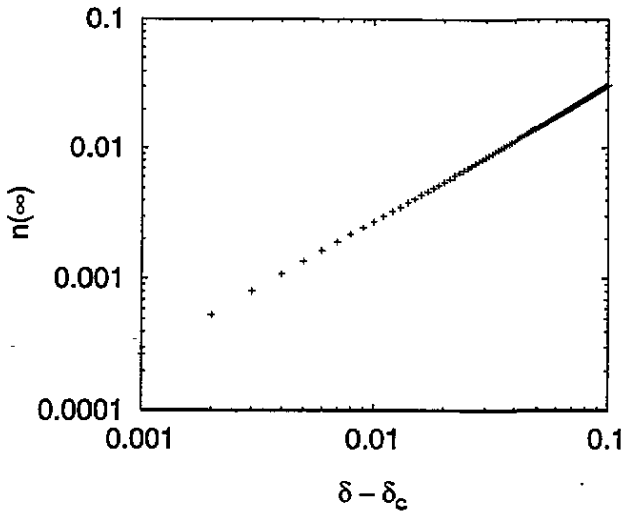
Figure 6. The $n = 3$ results of the GMF for $\rho(\infty)$ with $\Gamma = 0.35$ are shown on a double logarithmic plot as a function of $|(\delta - \delta_c)|$. The straight line gives $\beta = 1.0064$, which is used as a fictitious MF value in CAM.

Figure 5(*b*) shows the $n = 3, 4, 5$ results for $\Gamma = 0.05$, which are now compared with the $R = 1$ simulation data.

The critical exponent β of the order parameter has been determined by processing the results of the GMF approximation by the coherent-anomaly method (CAM) [14, 15]. According to CAM the GMF solution for kink density ρ at a given level of approximation—in the vicinity of the critical point δ_c—is the product of some mean-field behaviour multiplied by the anomaly factor $a(n)$:

$$\rho(n) = a(n) \, (\delta/\delta_c^n - 1)^{\beta_{MF}}. \tag{11}$$

The true critical exponent, β, can be obtained by fitting, using the knowledge that the divergence of the anomaly factor scales as

$$a(n) \sim (\delta_c^n/\delta_c - 1)^{\beta - \beta_{MF}} \tag{12}$$

as the level of approximation n goes to infinity. More precisely, for the available low level of approximations ($n \leqslant 6$), correction to scaling should also be taken into account

$$a(n) = b \, \Delta_n^{\beta - \beta_{MF}} + c \, \Delta_n^{\beta - \beta_{MF} + 1} + \cdots \tag{13}$$

where b and c are constants and the invariant variable

$$\Delta_n = (\delta_c/\delta_c^n)^{1/2} - (\delta_c^n/\delta_c)^{1/2} \tag{14}$$

is used. This new variable was introduced recently [15] to avoid the ambiguity on the choice of the independent variable ($\delta \leftrightarrow \delta^{-1}$). Using this new variable an accurate estimate was given for the critical exponents of the 3D Ising model [15] and for the exponent β of the stochastic rule 18 cellular automaton [20].

From our GMF approximation results, as shown on figure 3, we can use the $n = 4, 5, 6$ data for the CAM analysis, while the $n = 3$ result can be taken to represent the lowest-order MF approximation (with $\delta_c^{MF} = 0$) for a *continuous* transition (no jump in ρ for $n = 3$). For δ_c we use the results of the polynomial extrapolation. Figure 6 shows that in the $n = 3$ approximation the exponent $\beta = 1.0064$, thus $\beta_{MF} \approx 1$. Graphs similar to that in figure 6 have been obtained for $n = 4, 5, 6$ as well. Consequently, as table 1 shows, the anomaly factor does not depend on n. This means, according to (12), that the exponent is estimated to be equal to the 'mean-field' value $\beta \simeq \beta_{MF} = 1$.

Table 1. CAM calculation results.

n	Δ_c^n	$a(n)$
4	2.490 43	0.010 83
5	1.810 22	0.010 74
6	1.457 66	0.010 79

4. Discussion

Here the mean-field limit of the line of non-thermal phase transitions occurring in a family of one-dimensional kinetic Ising models has been analysed. This line consists of second-order Ising-to-active phase transition points which belong to the universality class found first by Grassberger *et al* [7, 8]. The first-order endpoint of this line has been found to be described by MF theory. Systematic generalized MF theory has been applied to treat bigger and bigger blocks of size n exactly in order to be able to depart from this tricritical point. Numerically solvable results up to $n = 6$ have given the support of simulation results, and especially have provided a value for the critical exponent β of the order parameter (density of kinks) $\beta = 1$, which is in accord with Grassberger's result: $\beta = 0.94 \pm 0.06$. The value $\beta = 1$ coincides with the MF β-exponent for directed percolation. This is not surprising in the case of our $n = 3$ result which we have used as an effective MF one for a *continuous* transition at $\delta = 0$. As Grassberger has pointed out [8] in the rate (or MF) approximation there is no difference between models leading to the Ising-to-active transition and directed percolation. In this argument, however, the MF equation is written for the kink density (and not for the magnetization as in (7)) and has the form: $d\rho/dt = 2\mu\rho - 2\lambda\rho^2$, where μ and λ are the reproduction and annihilation rates, respectively. Nevertheless, a heuristic equation of a similar type can also be constructed in the present model using $\mu \propto (p_{RW} - p_{an})$ as the rate making kink-reproduction effective (a conclusion stemming from simulations). The corresponding MF critical value is then $\delta_c^{MF} = 0$ and $\beta^{MF} = 1$. It is, however, surprising that higher-order approximations of GMF have given practically no deviation from the MF value of β. In simulations for branching annihilating random walk with four offspring, Jensen [9] conjectures a value $\beta = \frac{13}{14}$ on the basis of simulation results, no theoretical motivation appears to exist for this value, however. To decide the question of what the exact value of β is in this universality class appears to be a challenging task, and calculating GMF in even higher approximations than here would probably be worthwhile.

Acknowledgments

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