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Domain-growth properties of a two-dimensional kinetic Ising model

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Abstract. The domain-growth properties of the two-dimensional single spin-flip kinetic Ising model with a Metropolis-type transition function and checkerboard updating are investigated numerically with quenches from the high-temperature phase to temperatures in the ordered phase and to T_c. Measuring the structure factor $S(0,t) \propto t^{2x}$ and the autocorrelation function $A(t) \propto t^{-\tilde{\lambda}x}$ as a function of time, the effect of deterministic dynamics at $T = 0$ with $x = 1.0$ is followed throughout the ordered phase. At $T < T_c$, $T \not\approx T_c$, crossover from $x = 1.0$ to $x = 0.5$ is shown to occur with increasing time and even at $T = T_c$ the scaling exponents are still discernibly dependent on time. $\tilde{\lambda}$, however, is found to be unaffected in the whole temperature range.

1. Introduction

In the field of ordering kinetics one of the most interesting problems is the question of universality. It has long been clear that the conserved or non-conserved character of the order parameter plays an important role. Kinetic Ising models offer a useful laboratory for exploring the different factors which influence the scaling behaviour and the characteristic exponents of domain growth. The two-dimensional kinetic Ising model with Metropolis-type single spin-flip dynamics and checkerboard updating has been shown [1] to fall into a new universality class of domain growth for quenches from the high-temperature phase ($T = \infty$) to zero temperature. At $T = 0$ this model is deterministic and even the applied updating does not introduce any random element. This is the reason why the exponent x of the characteristic length scale $L(t) \propto t^x$ was found to be 1.0 in contrast to the usual (Allen–Cahn [2]) value 1/2 for a scalar non-conserved order parameter, obtainable with Glauber kinetics [3]. Numerical simulations have now been extended to temperatures up to T_c. Besides the structure factor we have measured the autocorrelation function, $A(t)$, the importance of which has only recently been recognized [4,5].

Concerning the characteristic length scale $L(t)$ and the domain-growth exponent, x, we have found that the characteristic time τ_0 connected with the rate of transition from determinicity, $w = \exp(-4J/kT)$, plays an important role as $\tau_0 \propto 1/w$. In the temperature–time plane τ_0 separates the 'phase diagram' into parts with $x = 1.0$ and $x = 1/2$ in such a way that, asymptotically, the latter dominates.

Further numerical evidence is provided here for the conjecture [5] that the exponent $\tilde{\lambda}$ in the expression $A(t) \propto t^{-\tilde{\lambda}x}$ is independent of the details of the dynamics, by showing that it is not influenced by the determinicity at $T = 0$ (the same is true at dimensionality one, in the same model, where x also equals 1.0, the ballistic motion is more striking [6]).

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At T_c the comparison between Metropolis and Glauber kinetics with checkerboard updating is analysed on the basis of simulation results.

We consider the ferromagnetic Ising model in a two-dimensional (2D) square lattice of size L with the Hamiltonian

$$H = \frac{-J}{kT} \sum_{i,j} s_i s_j \tag{1.1}$$

where the sum extends over the four nearest neighbours and $s_i = \pm 1$.

The dynamics of the Ising model is defined, as usual, via a stochastic interaction with the heat bath. The Metropolis transition rate [7] for flipping a spin at site i is given as

$$W_i = \min[1, \exp(-\Delta H)] \tag{1.2}$$

where $\Delta H = (2J/kT) s_i \sum_{nn} s_j$ is the energy needed for the flip; the sum runs over nearest neighbours. By applying this rule, checkerboard updating [8] is used. This circumstance gives rise to dynamics basically different from Glauber type dynamics due to its deterministic nature at zero temperature.

To investigate the time development of domain growth we consider the structure factor, $S(k, t)$, which is the Fourier transform of the equal-time correlation function $C(r, t)$,

$$C(r, t) = \left\langle \frac{1}{N} \sum_i s_i(t) s_{i+r}(t) \right\rangle \tag{1.3}$$

where the angular brackets denote averaging over initial conditions. The scaling forms of $S(k, t)$ and $C(r, t)$ are (see e.g. [5])

$$S(k, t) = L(t)^d g(kL(t)) \qquad C(r, t) = f(r/L(t)) \qquad L(t) \propto t^x \qquad \text{for } T \approx 0. \tag{1.4}$$

$L(t)$ is the characteristic length for quenches deep into the ordered phase; x is the domain-growth exponent. For quenches to T_c, critical scaling yields

$$S(k, t) = k^{-2+\eta} g_c(k\xi(t)) \qquad S(0, t) \propto \xi^{2-\eta}(t) \propto t^{\gamma/\nu Z} \tag{1.5}$$

with $\xi(t) \propto t^{1/Z}$, the non-equilibrium correlation length and $C(r, t) = r^{d-2+\eta} f_c(r/\xi(t))$. We shall also numerically study the autocorrelation function $A(t)$

$$A(t) = \left\langle \frac{1}{N} \sum_i s_i(t) s_i(0) \right\rangle \tag{1.6}$$

which is connected with the response to initial conditions (see [5]). $A(t)$ can also be written in scaling form:

$$A(t) \propto t^{-(d-\lambda)x} \equiv t^{-\tilde{\lambda}x} \qquad T \approx 0 \tag{1.7}$$

$$A(t) \propto t^{-(\lambda_c - d)/Z} \equiv t^{-\tilde{\lambda}_c/Z} \qquad T = T_c. \tag{1.8}$$

λ and λ_c are new exponents for dynamic correlations apparently independent of x and Z, respectively. For the 2D Ising model with Glauber kinetics $x = 0.5$, the value well known for a non-conserved scalar order parameter [2]. Moreover, $x_c = 7/8Z \approx 0.4$, using $\gamma/\nu = 1.75$ and $Z = 2.2$ [9, 10]. Concerning $\tilde{\lambda}$ and $\tilde{\lambda}_c$ Humayun and Bray [5] reported the following results for Monte Carlo simulations with Glauber kinetics: $\tilde{\lambda} = 1.24$ and $\tilde{\lambda}_c = 1.59 \pm 0.02$.

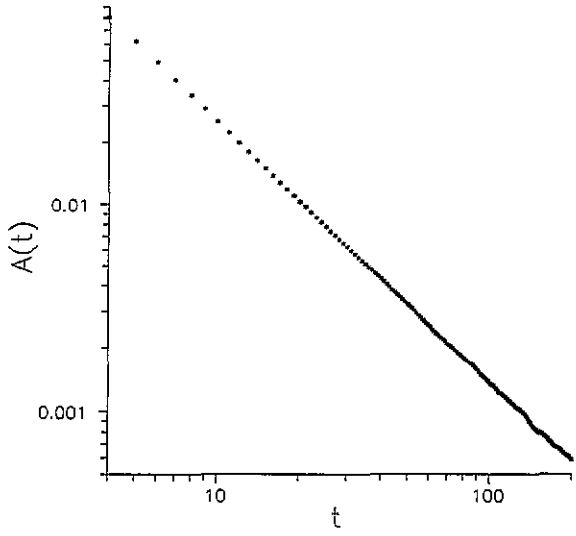

Figure 1. Log–log plot of the autocorrelation function at $T = 0$.

2. Simulations

Using the Hamiltonian, equation (1.1), and defining the dynamics of the Ising system through equation (1.2) plus prescribing synchronous checkerboard updating, simulations were performed for lattices of size $N = 50 \times 50$ to $N = 800 \times 800$, with periodic boundary conditions. In each case the system was started from a random distribution of spins ($T = \infty$). Statistical errors are everywhere up to about 10%.

2.1. Quench and equilibration at $T = 0$

In a previous paper [1] the author reported simulations of $S(0, t)$ and the excess energy density:

$$\Delta E(t) = \left\langle 1 - \frac{1}{4N} \sum_{nn} s_i s_j \right\rangle \propto t^{-y}.$$

The values obtained there were $x = y = 1.0$, in contrast to the standard values for the non-conserved order parameter, $x = y = 1/2$. In [1] it was also stressed that to see scaling, sufficiently large lattices have to be used: deterministic dynamics at $T = 0$ causes the development of flat domain walls which cannot change any further when $L(t) \propto t_0^x = L$ is reached; hence freeze-in of the domains sets in. Currently we are interested in finding the value of the exponent $\tilde{\lambda}x \approx \tilde{\lambda}$ of the autocorrelation function (1.7) to complete the above mentioned results. Data are presented for lattices of size 800×800 with averages over 1000 independent initial states. The least-mean-square fit to the data shown on figure 1 yields

$$\tilde{\lambda}^{\text{Metrop}} = 1.25 \pm 0.03$$

a value which agrees within the errors with that for Glauber dynamics ([5] and references therein). A small increase in the exponent with time has also been observed in the present simulations.

Data for the equal-time correlation function (1.3) is shown on figure 2 with r/t on the x axis. In spite of the relatively poor statistics, the data collapse onto a universal curve confirming the scaling form (1.4), and $L(t) \propto t$.

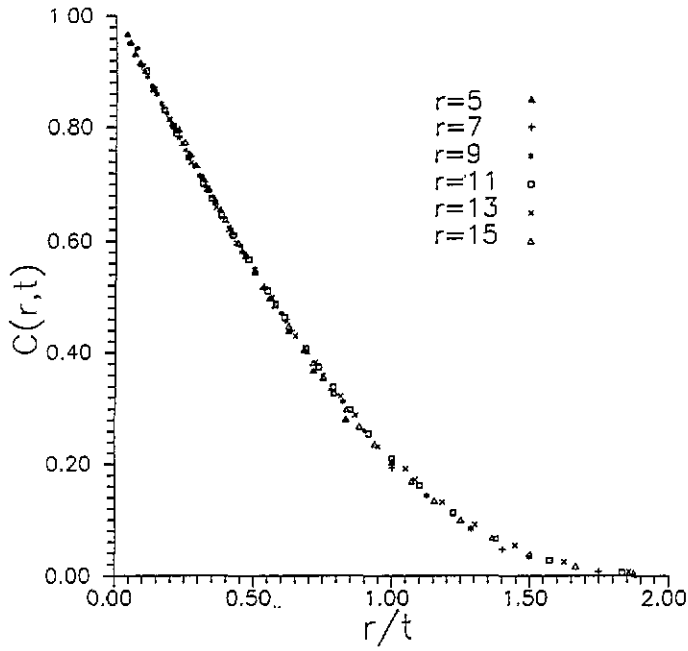

Figure 2. Equal-time correlation function for different values of the distance r: lattice size, $N = 200 \times 200$; number of independent initial states in the averaging, 250.

2.2. Quench and equilibration in intermediate temperatures

At $T \not\approx 0, T < T_c$, crossover from the $T = 0$ behaviour to Glauber-type behaviour is apparent in the time development of the domains. This feature is illustrated in figure 3, where numerical results for $S(0, t)$ are depicted for several values of the temperature in the ordered phase. Here $w = \exp(-4J/kT)$ emerges naturally as a measure of temperature; it is the transition rate from the deterministic ground state. T_c corresponds to $w = 0.1716$. Two characteristic times, τ_0 and τ_s, can be identified on the curves of figure 3 as the time of crossover and the time of saturation due to finite size, respectively. Below the crossover time the growth exponent is the same as that at zero temperature ($x = 1.0$); the magnitude of τ_0 is proportional to the inverse of the transition rate w, $\tau_0 \propto 1/w$, for $w \ll 1$, while the characteristic time of saturation is $\tau_s \propto L^{1/x}$ (see e.g. [11]). Thus, for example, for $L = 200$ and $w = 0.01$ no crossover regime can be seen before saturation sets in (curve b on figure 3). The effective growth exponent, i.e. the exponent of the best power-law fit in a given time interval, x_{eff}, between the two characteristic times, is expected to approach the Glauber value asymptotically if $L \to \infty$. For finite L, however, τ_s is determined by $x_{\text{eff}} \geqslant 0.5$. To calculate τ_s using $\tau_s = L^{1/x_{\text{eff}}}$, however, the first section of the time developmen' has to be taken into correction.

For fixed L, x_{eff} decreases with increasing w. Thus for $L = 200$, $x_{\text{eff}} = 0.71, 0.62$ and 0.50 for $w = 0.08, 0.1$ and 0.14, respectively (curves d, e and f on figure 3). Moreover, for given L and w, x_{eff} also has a slight time dependence; thus, for example, for $L = 800$, $w = 0.08$, x_{eff} is equal to 0.67, 0.62, 0.56, 0.53 and 0.50 in the intervals t =50–100, 100–200, 200–500, 500–800 and 700–800, respectively. As to the autocorrelation function $A(t)$, its exponent, $\tilde{\lambda}x_{\text{eff}}$ changes with w so that $\tilde{\lambda}$ remains at its zero-temperature value, within the error of the simulations. In the same runs as those above for $w = 0.08$, $L = 800$ for

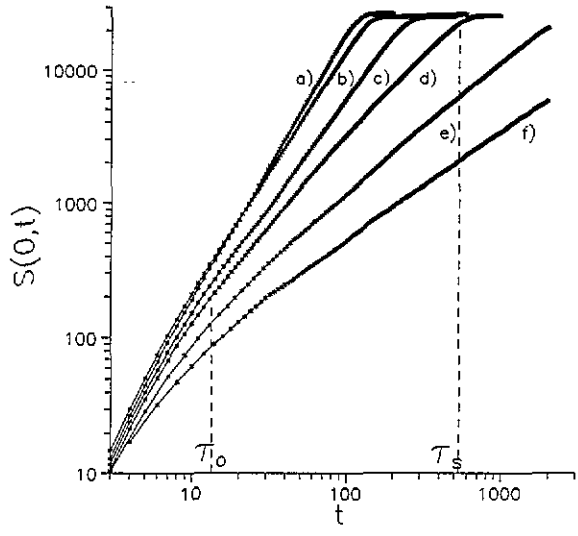

Figure 3. Structure factor as a function of time on a double-logarithmic scale for six values in the temperature range $0 \leqslant T \leqslant T_c$: (a)$w = 0$, (b)$w = 0.01$, (c)$w = 0.05$, (d)$w = 0.08$, (e)$w = 0.14$, (f) $w = 0.1716(T_c)$. τ_0 and τ_s refer to the curve (d). Lattice size: $N = 200 \times 200$; number of states in the averaging :1000, 500, 500, 500, 500 and 1800, respectively.

times up to $t = 800$ with averaging over 500 independent initial states we found $x_{\text{eff}} = 0.57$, $\tilde{\lambda}x_{\text{eff}} = 0.70$ between $t = 80$ and $t = 800$ yielding $\tilde{\lambda} = 1.2$. The time dependence here is: $\tilde{\lambda}x_{\text{eff}}$ changes in the time intervals as above like 0.69, 0.72, 0.70, 0.65 and 0.62, giving for $\tilde{\lambda}$ 1.0, 1.16, 1.26, 1.23 and 1.24, respectively. Similar behaviour has been found for $w = 0.05$, 0.1, 0.14 etc.

2.3. Quench and equilibration at T_c

For this quench we simulated lattices of size $N = 200 \times 200$ up to $t = 2000$; the corresponding curve for $S(0, t)$ is shown on figure 3(e). The effective exponent (best-fit value in a given time interval) in the interval of two decades is $2x_{\text{eff}} = 0.8$. The autocorrelation function, however, exhibits such large fluctuations for $t > 100$ that no conclusion could be drawn concerning its exponent. To find $\tilde{\lambda}_c$ another series of runs has been carried out for $L = 400$ and with averaging over 10^4 independent random initial states, in the interval $t = 1$–200. Our results are shown in figure 4, where $S(0, t)$ and $[A(t)]^{-1}$ are depicted on a double-logarithmic scale. Power-law behaviour can be identified but with somewhat time-dependent exponents. At $T = T_c$ equations (1.5) and (1.8) are expected to be valid. Effective Z values can also be deduced through $2x_c = \gamma/\nu Z$. The best-fit exponents together with the corresponding Zs are shown in table 1. These values (considering time dependences, too) are in accord with those reported recently by Ito [10] for the the Metropolis transition rate with checkerboard updating through a finite-size scaling formula for the decay of magnetization in the limit $N \to \infty$.

The inverse of the autocorrelation function as a function of time is also shown in figure 4, on a double-logarithmic scale. The exponent again exhibits slight changes with temperature: the third column of table 1 shows the best-fit values in different time intervals and values of L.

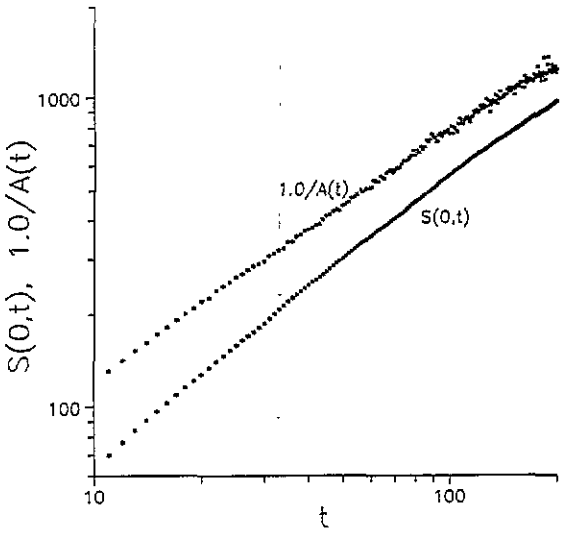

Figure 4. Plot of $S(0,t)$ and $A(t)^{-1}$ on a double-logarithmic scale. Data are averaged over 10^4 histories of a 400×400 system.

Table 1. Best-fit exponents of $S(0,t)$ and $A(t)$ at $T = T_c$. For $L = 200$ the number of states averaged is 1800; here, due to fluctuations, the autocorrelation function could be evaluated only up to $t = 200$. For $L = 400$ the data from figure 4 have been used. In column 4, the value of Z deduced from $2x_c = 7/4Z$ is given in parentheses while column 5 contains the $\tilde{\lambda}_c$s obtained from results in column 3 with Zs in column 4.

Time interval	$2x_c$	$\tilde{\lambda}_c/Z$	Z	$\tilde{\lambda}_c$
20–2000($L = 200$)	0.80	—	(2.2)	—
20–200($L = 200$)	0.85	0.75	(2.1)	(1.6)
20–200($L = 400$)	0.86	0.78	(2.0)	(1.6)
Value in [5] for Glauber MC	0.81	0.74	(2.16)	(1.6)

It is apparent that the obtained data, asymptotically and within the error of simulations, agree with those reported for Glauber kinetics [5]. This fact is not surprising as the crossover results in the preceding section have already indicated that in the asymptotic regime and at finite temperatures the differences between Metropolis and Glauber kinetics disappear.

We have made simulations at $T = T_c$ for Glauber kinetics with checkerboard updating to check for differences at earlier times. For lattices of size 400×400 and with averages over 3500 independent initial conditions our results show that in the time intervals $t = 10$–50, 50–100 and 100–200, $2x_c$ takes the best-fit values of 0.85, 0.83 and 0.82, respectively, while in the Metropolis case (for $L = 400$, 10^4 averages) $2x_c$ changes in the same intervals to 0.96, 0.89 and 0.78, respectively. Thus in the Glauber case, in spite of the lower (1/3) number of independent states in the averaging over initial conditions, there is much (five times) less change with time in the effective exponents. It is apparent that Glauber kinetics is much less sensitive to size effects.

We have also checked the scaling behaviour of the equal-time correlation function (1.5); the result is shown in figure 5, where $C(r,t)r^{1/4}$ is depicted with the abscissa being the scaling variable $r/t^{1/Z}$, using $Z = 2.1$.

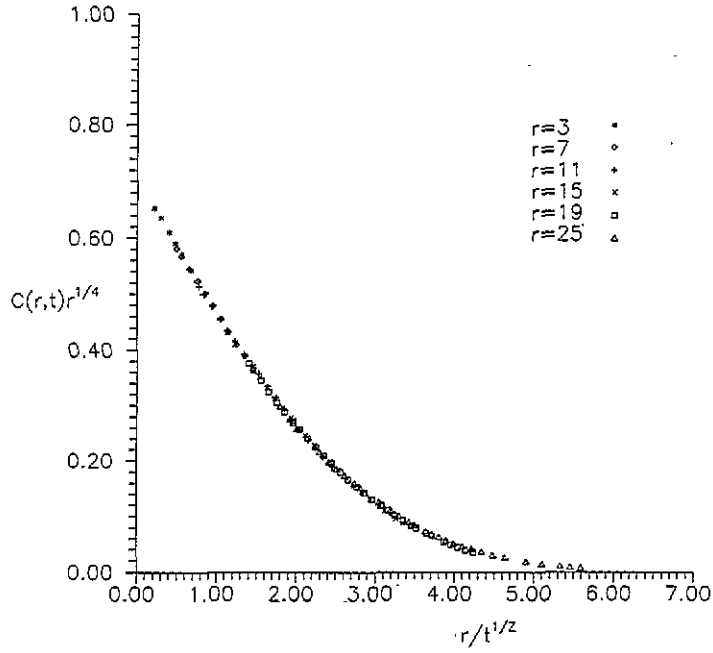

Figure 5. Scaling plot of the equal-time correlation function for quenching from $T = \infty$ to $T = T_c$: system size, 400×400; number of states in the averaging, 750.

3. Discussion

The growth properties of the two-dimensional single spin-flip kinetic Ising model with a Metropolis-type transition function and checkerboard updating have been investigated numerically. The ferromagnetic structure factor and the autocorrelation function as a function of time have been studied at different temperatures below T_c and at T_c. It is usually stressed [5, 12] that domain growth in the ordered phase is dominated by the $T = 0$ fixed point in the framework of a renormalization group calculation. In the case investigated here the limits $T \to 0$ and $t \to \infty$ are not interchangeable: at $T = 0$, $t \to \infty$ $x = 1.0$ while for any $T \neq 0$, $T < T_c$, and $t \to \infty$ Allen–Cahn-type behaviour sets in, in the thermodynamic limit. For finite times and L, crossover between these two types of behaviour is observed with exponent $x_{\text{eff}} \geqslant 1/2$, which decreases with increasing w for fixed L.

At T_c our motivation has been to see whether some behaviour reminiscent of that in the time development of growth is still present or whether it now follows Glauber kinetics. We have found discernible differences between Glauber and Metropolis kinetics with checkerboard updating for the quantities investigated here in the non-asymptotic regime unfavourably to the latter. Much bigger (finite-size) fluctuations especially in the autocorrelation function and larger time dependences in the effective growth exponent characterize simulations with the Metropolis model in comparison with the Glauber one. The present investigations suggest that the 'bad nature' of the Metropolis case can be traced back to its determinicity at zero temperature with the corresponding crossover behaviour for finite values of T. These findings offer an explanation for the simulation results reported recently for the critical dynamical exponent Z by Ito [10], who found pronounced differences in the way the (apparently universal) asymptotic value ($L \to \infty$, $t \to \infty$) is approached for the two models mentioned above.

By measuring the exponent of the autocorrelation function $\tilde{\lambda}$ in the whole interval $0 \leqslant T < T_c$ we have provided a further check and support, at least for the case of initial conditions with short-range correlations, for the idea [5] that $\tilde{\lambda}$ is unrelated to the exponent describing the growth of domains with time. Analytical confirmation exists only for the case $n \to \infty$ [12], where n is the number of components of the order parameter. The effect of crossover, being connected with the motion of domain walls only, was practically (i.e. within the errors of simulations) unobservable in $\tilde{\lambda}$.

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References

[1] Menyhárd N 1990 *J. Phys. A: Math. Gen.* **23** 5109
[2] Allen M and Cahn J W 1979 *Acta Metall.* **27** 1085
[3] Glauber R J 1963 *J. Math. Phys.* **4** 294
[4] Janssen H K, Schaub B and Schmittmann B 1989 *Z. Phys.* **73** 539
[5] Humayun K and Bray A J 1991 *J. Phys. A: Math. Gen.* **24** 1915
[6] Menyhárd N 1990 *J. Phys. A: Math. Gen.* **23** 2147
[7] Metropolis N, Rosenbluth A W, Rosenbluth M N, Teller A H and Teller E 1953 *J. Chem. Phys.* **21** 1087
[8] Vichniac G Y 1984 *Physica* **10D** 96
Pomeau Y 1984 *J. Phys. A: Math. Gen.* **17** L415
[9] Münkel Ch, Heermann D W, Adler I, Gofman M and Stauffer D 1993 *Physica* **193A** 540
[10] Ito N 1993 *Physica* **192A** 604; **196A** 591
[11] Milchev A, Binder K and Heermann D W 1986 *Z. Phys.* B **63** 521
[12] Newman T J and Bray A J 1990 *J. Phys. A: Math. Gen.* **23** L279