Determination of the dynamic critical exponent by quench kinetics simulations

G. Besold, W. Schleier, and K. Heinz
Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstrasse 7, D-91058 Erlangen, Federal Republic of Germany
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A two-dimensional lattice-gas model was quenched from a disordered state to the maximum critical temperature of a 2×1 superstructure and its ordering kinetics studied by Monte Carlo simulation. The critical growth exponent n_c was determined from the time evolution $\langle\Psi^2\rangle_t \sim t^{2n_c}$ of the scalar 2×1 order parameter Ψ. The relation $z=(2-\eta)/2n_c$ (with static critical exponent $\eta=\frac{1}{4}$) was then applied to evaluate the (linear) dynamic critical exponent z. With Kawasaki dynamics the exact value $z=2$ of model C of critical dynamics (nonconserved order parameter, conserved density) was recovered whereas a value $z=2.19\pm0.04$ resulted for model A (nonconserved order parameter *and* density) with Glauber dynamics.

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The dynamic critical exponent z of the two-dimensional spin-flip Ising model is not known exactly yet, despite many attempts which have been made in the past to solve this problem. The dynamic critical exponent describes the divergence of the relaxation time τ near the critical point according to $\tau\sim|T-T_c|^{-\nu z}$, where T_c is the critical temperature and ν the static critical exponent of the correlation length. A variety of different techniques has been applied to determine z, including, e.g., time correlation matching with Monte Carlo renormalization group (MCRG) methods [1–6], relaxation measurements on critically equilibrated systems (including finite-size scaling) [7–16], recording of "damage spreading" in spin systems subsequent to a localized initial perturbation [17–19], and high-temperature series expansions [20–24]. However, the results (which are compiled, e.g., in Ref. [6]) are not fully consistent with each other and typically range from slightly below 2.0 to slightly above 2.2. Recent estimates are $z=2.13\pm0.01$ (MCRG calculations [6]), $z=2.18\pm0.03$ (large-scale Monte Carlo simulations on a parallel computer [16]), and $z=2.183\pm0.005$ (high-temperature series expansions up to 20th order [24]).

In this paper we present results from quench kinetics simulations of a 2D lattice-gas model which—as an independent method—allow an estimate for the linear dynamic critical exponent z as well. Generally, the method works as follows: At time $t=0$ the system is quenched from a totally disordered state (corresponding to infinitely high temperature) to a critical point of an ordered phase with order parameter Ψ (which was scalar in this case, see details given below). After a short transient the average linear size $R(t)$ of ordered domains is expected to grow with time according to a power law

$$R(t)\sim\sqrt{\langle\Psi^2\rangle_t}\sim t^{n_c} \tag{1}$$

with a "critical" growth exponent n_c ($\langle\ \rangle_t$ denotes an ensemble average at time t). Here the root mean square of the order parameter Ψ is used as a measure for the average domain size $R(t)$. The power law (1) will be valid as long as time is small compared to the relaxation time τ. To be precise, τ is the *linear* relaxation time (and z the *linear* dynamic critical exponent), since the equilibrium values of the order parameter both before and after the quench (at $T=\infty$ and $T=T_c$, respectively) are equal (zero), at least for a system of infinite size. Dynamic scaling assumptions lead to the relation [25–27]

$$z=\frac{2-\eta}{2n_c} \tag{2}$$

between the critical growth exponent n_c and the dynamic critical exponent z, including the static critical exponent η which is known exactly for the two-dimensional (2D) Ising universality class ($\eta=\frac{1}{4}$). Monte Carlo simulation of domain growth at $T=T_c$ therefore allows the determination of z from the observed critical growth exponent n_c. Using this method Huse [25] derived the estimate $z=2.16\pm0.03$ for the spin-flip Ising model on a 57×57 square lattice. The method was proposed by Binder and co-workers [26–30] also as a promising technique for an experimental determination of z for chemisorbed overlayers (where the domain growth process can be monitored by the time evolution of diffraction spot intensities, i.e., the equal-time structure factor). However, to our knowledge, this has not been done yet.

In our simulation study we considered a lattice gas on a rectangular lattice with $\sqrt{N}\times\sqrt{N}$ sites, periodic boundary conditions, and grand canonical model Hamiltonian

$$H=-\varepsilon_x\sum_{\langle i,j\rangle_x}c_ic_j-\varepsilon_y\sum_{\langle i,j\rangle_y}c_ic_j-\mu\sum_{i=1}^{N}c_i\ ,$$
$$c_i,c_j\in\{0,1\}\ , \tag{3}$$

where the interaction parameter ε_x between the occupied nearest-neighbor (NN) sites i,j in the x direction was arbitrarily chosen to be *repulsive* ($\varepsilon_x<0$) and the NN interaction ε_y in the y direction *attractive* ($\varepsilon_y>0$) with the ratio $\varepsilon_x:\varepsilon_y=-1:3$. The last term in Eq. (3) containing the chemical potential μ is the energy contribution of the occupied sites. It is absent if the canonical ensemble with fixed coverage $\theta=(1/N)\langle\sum_i c_i\rangle$ is used. With only pairwise interactions considered the temperature vs coverage

phase diagram of this simple model is symmetric with respect to coverage $\theta=0.5$. It exhibits a single ordered phase with a 2×1 superstructure corresponding to alternating occupied and empty columns of lattice sites [31, 32]. The transition from the disordered to the 2×1 phase is continuous with a scalar order parameter $\Psi(\{c_{ij}\}) := (2/N)\sum_i\sum_j(-1)^j c_{ij}$ (where i,j now denote row and column indices, respectively). Our computer simulations were performed for a lattice of $N=64\times64$ sites. For a chemisorption system this is comparable to typical terrace sizes on nominally flat low-index metal surfaces. For this finite system size the maximum critical temperature $T_c^{\max}=T_c(\theta=0.5)=0.349\pm0.001$ in units of ε_y/k_B was determined in a previous study of equilibrium properties of the model [31].

It should be pointed out that both the critical growth exponent n_c and the resulting dynamic critical exponent z may belong to different universality classes of critical dynamics, depending on whether the canonical or the grand canonical ensemble is used. If Glauber dynamics with "inversion" of the occupation state $c_{ij}\rightarrow1-c_{ij}$ is applied (corresponding to ordering via adsorption-desorption processes), then the chemical potential has to be held constant and both the coverage and the order parameter are not conserved during the simulation. The dynamics of the model then corresponds to the spin-flip dynamics of the Ising model and belongs to the universality class of "model A" in the Hohenberg-Halperin classification of critical dynamics [33]. If, on the other hand, Kawasaki dynamics (particle-hole exchange between nearest neighbors in the x or y direction) is applied, then the order parameter remains not conserved but is coupled to a conserved quantity, the coverage θ. The dynamics then belongs to the class of "model C", for which z is known to have the exact value $z=2$ [33]. (In contrast, the dynamics of the spin-exchange Ising model belongs to the class of "model B" with conserved order parameter.) So, simulations using Kawasaki dynamics allow an accuracy check of the quench kinetics method for the determination of z. The simulational procedures and results using Kawasaki dynamics are reported below.

Before each quench the lattice was prepared in a completely disordered state ($\langle\Psi^2\rangle_{t=0}\approx0$) at coverage $\theta=0.5$. In order to check the sensitivity of the method, the system was quenched to $T_c^{\max}$ as well as to temperatures both slightly below and above this value. For every final quench temperature 1000 independent Monte Carlo (MC) simulations up to $t=5000$ Monte Carlo steps per site (MCS) have been performed on a CRAY Y-MP supercomputer to evaluate time-dependent averages $\langle\Psi^2\rangle_t$. We used a special MC algorithm ("hybrid algorithm") which was developed to speed up superstructure domain growth simulations by partial vectorization. It has been demonstrated in extensive tests that our algorithm suppresses vectorization-induced artificial spatial correlations across the lattice to a negligibly low level. The results yielded are in excellent agreement with those from conventional serial algorithms [31,32,34].

For each quench temperature the resulting data $\langle\Psi^2\rangle_t$ were analyzed in terms of a time-dependent effective growth exponent

$$n_{\text{eff}}(t)=\tfrac{1}{2}\frac{d[\ln\langle\Psi^2\rangle_t]}{d[\ln t]}\ . \tag{4}$$

In order to reduce roughening effects associated with numerical differentiation, $n_{\text{eff}}(t)$ was determined from the slope of lines fitted to each group of 25 successive data points centered at t in a plot of $\log\langle\Psi^2\rangle_t$ vs $\log t$. The results are shown in Fig. 1 as a function of time for five different quench temperatures T. For $T\le T_c^{\max}=0.349$ [Figs. 1(a)–(c)] the following common features can be observed with increasing time: (1) an initial period with n_{eff} decreasing which lasts longer the higher T is chosen (up to $t\approx500$ MCS at $T_c^{\max}$); (2) an almost constant level (apart from some residual wiggles caused by statistical fluctuations) which, however, decreases and also persists longer in time with increasing temperature; (3) finally, a further continuous reduction of n_{eff} which is associated with a crossover to saturation of $\langle\Psi^2\rangle$ at its equilibrium value. Obviously the intermediate constant level of n_{eff} must be interpreted as the growth exponent $n(T)$ in a generalization of Eq. (1) to $T<T_c$ [with $n_c\equiv n(T_c^{\max})$]. For $T=0.3494$ [Fig. 1(d)], which is above but still within the $\pm1\sigma$ range 0.348–0.350 of our estimate of $T_c^{\max}$, the intermediate period with a constant level of n_{eff} is already considerably reduced. It has completely disappeared at

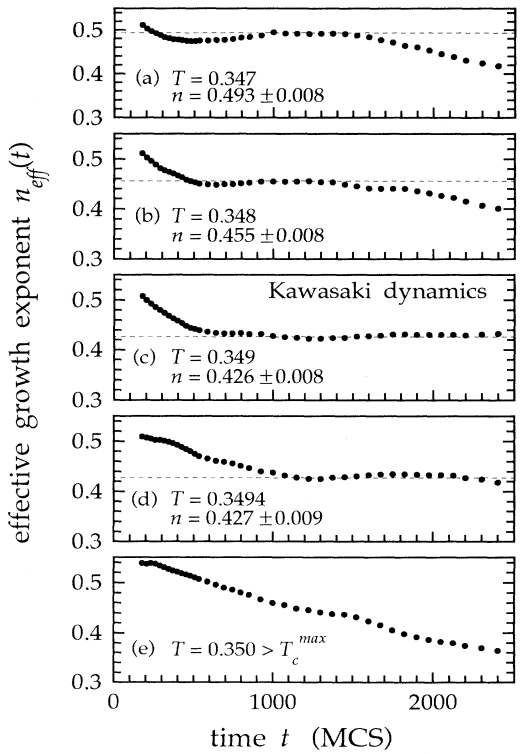

FIG. 1. Effective growth exponent $n_{\text{eff}}(t)$ as a function of time for different quench temperatures T derived from averages over 1000 independent MC runs with Kawasaki dynamics (system size 64×64): (a) and (b), $T<T_c^{\max}$; (c) and (d), $T\approx T_c^{\max}$; and (e), $T>T_c^{\max}$. The resulting growth exponents $n(T)$ are shown as insets.

$T=0.350$ [Fig. 1(e)] where n_{eff} decreases more or less continuously over the whole time range. It is obvious that $T_c^{\max}<0.350$, which can be taken as an *a posteriori* verification that our previously determined estimate $T_c^{\max}\approx 0.349$ is consistent with the findings from growth kinetics.

For each quench temperature $T\le T_c^{\max}$ the growth exponent $n(T)$ was evaluated by fitting a power law to up to 55 points of the original $\langle\Psi^2\rangle_t$ data within the intermediate time regime within which $n_{\text{eff}}(t)$ is almost constant. The resulting numerical values for n are shown as inserts in Figs. 1(a)–1(d). At $T=0.347\approx 0.994T_c^{\max}$, the fit leads to $n=0.493\pm 0.010$ which is still in excellent agreement with the prediction $n=0.5$ from the Lifshitz-Allen-Cahn theory of curvature-driven domain growth [35,36]. In a previous study also lower quench temperatures down to $0.6T_c^{\max}$ were considered and in all cases the growth exponent turned out to be very close to $n=0.5$ [31,32]. At $T=0.348\approx 0.997T_c$, n has decreased to $n=0.455\pm 0.010$, and for $T=0.349\approx T_c^{\max}$ the value $n\approx n_c=0.426\pm 0.010$ results (and almost the same value 0.427 ± 0.010 for $T=0.3494$). From Eq. (2) we then find the estimate $z=:z_C=2.05\pm 0.05$ for "model C" which agrees with the exact value $z_C=2$ within the $\pm 1\sigma$ range. We expect a comparable accuracy in the case where the method is used with Glauber dynamics, which we discuss next.

With Glauber dynamics the procedures of simulation and data reduction were the same as in the case of Kawasaki dynamics, except that now the chemical potential was fixed at its "critical" value $\mu=\mu_c=-\frac{2}{3}$ (corresponding to zero magnetic field of the isomorphic superantiferromagnetic spin model with 2×1 superstructure). In contrast to the simulations with Glauber dynamics the ordering proceeds faster and finite-size effects cannot be neglected already above $t\approx 700$ MCS. In Fig. 2 the root-mean-square order parameter derived from 1300 independent MC runs is shown as a function of time at $T_c^{\max}=0.349$ A power law has been fitted in the time interval 40–600 MCS with a resulting critical growth exponent $n_c=0.399\pm 0.007$. This fit value turned out to be quite stable (up to changes in the last decimal) with respect to minor modifications of position and size of the time interval used for the fit. Using Eq. (2) this leads to the estimate $z=:z_A=2.19\pm 0.04$ for the dynamic critical exponent of model A.

Within the error limits this agrees well with previous results $z=2.18\pm 0.03$ from Monte Carlo autocorrelation time measurements [16] and $z=2.16\pm 0.03$ from quench kinetic simulations of the Ising model [25] where averages over more than 50 000 MC runs for a square lattice of similar size 57×57 were used explaining the slightly smaller error bounds compared to our result. Our estimate for z is remarkably close to the value $z=2.183\pm 0.005$ derived from high-temperature series expansion calculations recently [24], although the error bars of our result are larger by almost an order of magnitude.

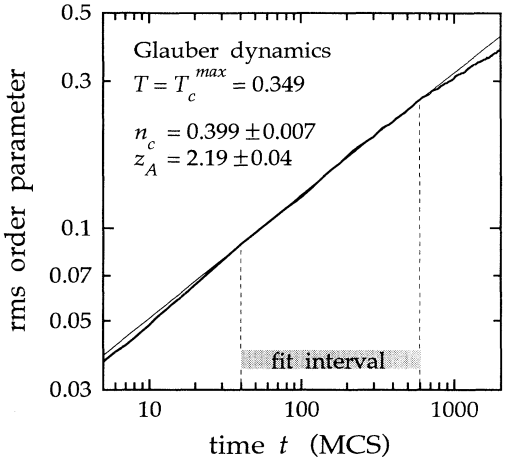

FIG. 2. Time evolution of the root-mean-square order parameter $\sqrt{\langle\Psi^2\rangle_t}$ at $T=T_c^{\max}=0.349$ after averaging over 1300 independent MC runs with Glauber dynamics (system size 64×64). The thick solid line represents the MC data and the thin solid line the power law with exponent n_c fitted in the time interval 40–600 MCS. Both n_c and the resulting value for $z\equiv z_A$ are shown as insets.

To summarize, we have evaluated the dynamic critical exponent $z_A=2.19\pm 0.04$ of model A from quench kinetics simulation with Glauber dynamics at T_c of a lattice-gas model with 2×1 superstructure. Despite the only moderately large lattice size and number of MC runs used for averaging, our result agrees remarkably well with a recent estimate from high-temperature series expansions. The accuracy of our result could be checked independently by performing quench kinetics simulations also with Kawasaki dynamics, leading to the estimate $z_C=2.05\pm 0.05$ for model C which is close to the exact value $z_C=2$. High-precision estimates for z can be expected if the number of independent MC runs used for averaging will be increased further by at least two orders of magnitude. However, our results already demonstrate that quench kinetics simulation at T_c is a promising alternative method for the determination of the dynamic critical exponent z.

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