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PHASE ORDERING DYNAMICS OF ϕ^4-THEORY WITH HAMILTONIAN EQUATIONS OF MOTION

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Phase ordering dynamics of the $(2+1)$- and $(3+1)$-dimensional ϕ^4-theory with Hamiltonian equations of motion is investigated numerically. Dynamic scaling is confirmed. The dynamic exponent z is different from that of the Ising model with dynamics of model A, while the exponent λ is the same.

1 Introduction

It is believed that macroscopic properties of many particle systems could, in principle, be described by microscopic deterministic equations of motion (e.g. Newton, Hamiltonian, and Heisenberg equations), if all interactions, boundary conditions, and initial states could be taken into account. In practice, however, it is very difficult to solve these equations, except for some simple cases. Therefore, statistical mechanics was developed to deal effectively with such systems. Usually, ensemble theories are appropriate for equilibrium states, but they are inadequate for non-equilibrium states, where a general theory does not exist. In many cases, stochastic dynamics, e.g. following from Langevin-type equations of motion or Monte Carlo dynamics, are approximate theories. Anyway, it is an open question whether microscopic equations of motion could really produce the results of statistical mechanics, or vice versa (see Refs. [1–5]).

With the development of computers, it becomes gradually more and more possible to solve microscopic deterministic equations *numerically*. This at-

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tracts scientists of different fields. The study of microscopic fundamental dynamics aims on the one hand to test statistical mechanics, and on the other hand to explore new physics. For example, if a system is isolated, there is only internal interaction, and periodic boundary conditions can be adopted. So, computations are greatly simplified. To achieve ergodicity, the system should start from random initial states. Recently, such effort has been made for the $O(N)$ vector model and XY model [5–7]. The results support that deterministic Hamiltonian equations correctly describe second-order phase transitions. The estimated static critical exponents are consistent with those calculated from canonical ensembles (e.g. see the recent text book [8]). More interestingly, the macroscopic short-time (non-equilibrium) dynamic behavior of the $(2+1)$-dimensional ϕ^4-theory at *criticality* has also been investigated and dynamic scaling is found [9,10]. The results indicate that Hamiltonian dynamics in two dimensions with random initial states is in the same universality class of Monte Carlo dynamics of model A.

In a similar spirit, phase ordering dynamics of the $(2+1)$-dimensional ϕ^4-theory with Hamiltonian equations of motion has been investigated in Ref. [11] Assuming random initial states, there is a minimum energy density which is above the real minimum energy density of the system. Starting from this minimum energy density (note that energy is conserved), which is well below the critical energy density, phase ordering occurs. Dynamic scaling behavior is found. The dynamic exponent z is different from that of model A dynamics, but the exponent λ governing the power-law decay of the autocorrelation looks the same. It is somewhat interesting that the scaling function of the equal-time spatial correlation function is the same as that of the Ising model with model A dynamics. All results are independent of the parameters in the system.

The purpose of this article is twofold: Firstly, we generalize the computations to $(3+1)$ dimensions, which is important because our realistic world is in $(3+1)$ dimensions. Furthermore, in phase ordering of model A dynamics, the dynamic exponent z is dimension-independent but the exponent λ is dimension-dependent. It is interesting to see whether this property is kept in Hamiltonian dynamics. Attention will also be put on whether the scaling function of the equal-time spatial correlation function in three dimensions is the same as the one of the Ising model with model A dynamics. Secondly, to achieve more confidence on our conclusions, we will reexamine the results for $(2+1)$ dimensions obtained in Ref. [11], using somewhat different, more careful approaches. Since the computations in $(3+1)$ dimensions are very

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time consuming, more accurate data are obtained in $(2+1)$ dimensions.

2 Phase Ordering Dynamics

In the following, we outline phase ordering dynamics with Hamiltonian equations of motion. For a recent review of general ordering dynamics, readers are referred to Ref. [12].

2.1 The Model

For an isolated system, the Hamiltonian of the $(d+1)$-dimensional ϕ^4-theory on a square or cubic lattice is

$$H = \sum_i \left[\frac{1}{2}\pi_i^2 + \frac{1}{2}\sum_\mu (\phi_{i+\mu} - \phi_i)^2 - \frac{1}{2}m^2\phi_i^2 + \frac{1}{4!}g\phi_i^4 \right] \tag{1}$$

with $\pi_i = \dot{\phi}_i$. It leads to the equations of motion

$$\ddot{\phi}_i = \sum_\mu (\phi_{i+\mu} + \phi_{i-\mu} - 2\phi_i) + m^2\phi_i - \frac{1}{3!}g\phi_i^3 \ . \tag{2}$$

Here μ represents spatial directions and energy is conserved in these equations. The solutions are supposed to generate a microcanonical ensemble. The temperature could be defined as the averaged kinetic energy. For the *non-equilibrium* dynamic system, however, total energy is a more convenient controlling parameter, since it is conserved and can be taken as an input from initial states. For given parameters m^2 and g, there exists a critical energy density ϵ_c, separating the ordered phase (below ϵ_c) and the disordered phase (above ϵ_c). The phase transition is of second order.

We should emphasize that a Langevin equation at zero temperature is also "deterministic" in the sense that there is no noise. But it is essentially different from the Hamiltonian equations (2). The former describes relaxation towards equilibrium at zero temperature for a non-isolated system, but the latter contains full physics at all temperatures for an isolated system.

The order parameter of the ϕ^4-theory is the magnetization. The time-dependent magnetization $M \equiv M^{(1)}(t)$ and its second moment $M^{(2)}$ are defined as

$$M^{(k)}(t) = \frac{1}{L^{dk}} \left\langle \left[\sum_i \phi_i(t) \right]^k \right\rangle, \quad k = 1, 2. \tag{3}$$

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L is the lattice size and d is the spatial dimension. Here, the average is *over initial configurations*, which means that it is a real sample average and different from the time average in equilibrium. Following ordering dynamics with stochastic equations [12], we consider the dynamic process that the system, initially in a *disordered* state but with an energy density well below ϵ_c, is suddenly released to evolve according to Eq. (2). For simplicity, we set the initial kinetic energy to zero, i.e. $\dot{\phi}_i(0) = 0$. To generate a random initial configuration $\{\phi_i(0)\}$, we first fix the magnitude $|\phi_i(0)| \equiv c$, then randomly give the sign to $\phi_i(0)$ with the restriction of a fixed magnetization in units of c, and finally the constant c is determined by the given energy. In case of stochastic dynamics, scaling behavior of phase ordering is dominated by the fixed point $(T_I, T_F) = (\infty, 0)$ with T_I being the initial temperature and T_F being the temperature after quenching [12]. In Hamiltonian dynamics, the energy density cannot be taken to the real minimum $e_{\min} = -3m^4/2g$ since the system does not move. Actually, for the initial states described above, the energy is given by

$$V = \sum_i \left[(d - \frac{1}{2}m^2)\phi_i^2 + \frac{1}{4!}g\phi_i^4 \right] \ . \tag{4}$$

For the case of $d < m^2/2$ phase ordering occurs when the initial magnetization is set to zero for an energy density well below the critical point ϵ_c, due to the competition of two ordered states [11]. The scaling behavior is dominated by the minimum energy density $v_{\min} = V_{\min}/L^d$, which is a kind of fixed point. Above $v_{\min}$, there are extra corrections to scaling. From now, we redefine the energy density $e_{\min}$ as zero. Then the fixed point is $\epsilon_0 = v_{\min} - e_{\min}$. In this article, we consider only the energy density at exactly the fixed point ϵ_0.

2.2 Dynamic Scaling Behavior

Let us first consider the case of the initial magnetization $m_0 = 0$. An important observable is the equal-time correlation function

$$C(r,t) = \frac{1}{L^d} \left\langle \sum_i \phi_i(t)\phi_{i+r}(t) \right\rangle \ . \tag{5}$$

The scaling hypothesis is that, at the *late* stage of the time evolution, $C(r,t)$ obeys the scaling form

$$C(r,t) = f(r/t^{1/z}) \ , \tag{6}$$

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where z is the so-called dynamic exponent. Here, "late" is meant in a microscopic sense. In other words, when the domain size ($\sim t^{1/z}$) is big enough in units of the lattice spacing, scaling behavior emerges. At finite t, of course, there may be corrections to scaling which are generally not universal. They may induce difficulties for observing scaling behavior and uncertainties in the determination of the critical exponents.

Simple understanding of the scaling behavior of $C(r,t)$ can be achieved from the second moment of the magnetization. Integrating over r in Eq. (6), we obtain the power law behavior

$$M^{(2)}(t) \sim t^{d/z} \ . \tag{7}$$

Another interesting observable is the auto-correlation function

$$A(t) = \frac{1}{L^d} \left\langle \sum_i \phi_i(0)\phi_i(t) \right\rangle . \tag{8}$$

The scaling hypothesis leads to the power law

$$A(t) \sim t^{-\lambda/z}, \tag{9}$$

which implies that ordering dynamics is in some sense "critical". Here λ is another independent exponent.

For the discussions above, the initial magnetization m_0 is set to zero. If m_0 is non-zero, the system reaches a unique ordered state within a finite time. If m_0 is infinitesimally small, however, the time for reaching the ordered state is also infinite and scaling behavior can still be expected, at least at relatively early times (in a macroscopic sense). In this case, an interesting observable is the magnetization itself. It increases by a power law

$$M(t) \sim t^{\theta}, \quad \theta = (d-\lambda)/z. \tag{10}$$

The exponent θ can be written as x_0/z, with x_0 being the scaling dimension of m_0. This power-law behavior has been investigated in critical dynamics [13,14]. The interesting point here is that θ is related to the exponent λ which governs the power-law decay of the auto-correlation. By combining measurements of θ and λ, one can also estimate the dynamic exponent z.

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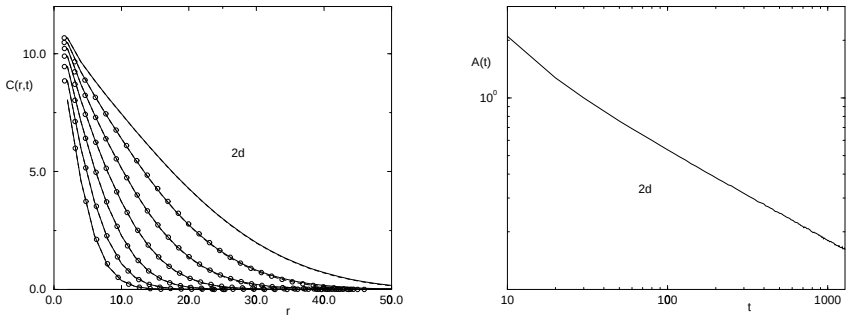

(*a*) (*b*)

Figure 1. (a) $C(r,t)$ in two dimensions obtained with $L = 256$ and $\Delta t = 0.01$ is plotted with solid lines for $t = 20$, 40, 80, 160, 320, 640, and 1280 (from left). Circles fitted to the curve at the time t indicate the data at the time $2t$ with r being rescaled by a factor $2^{-1/z}$. $C(r,t)$ obtained with $\Delta t = 0.02$ is also plotted with dashed lines. These overlap almost completely with the solid lines. (b) $A(t)$ obtained with $\Delta t = 0.01$ (the solid line) on a log-log scale. The curve for $\Delta t = 0.02$ overlaps completely with that for $\Delta t = 0.01$.

3 Numerical Results

To solve the equations of motion (2) numerically, we discretize $\ddot{\phi}_i$ by $[\phi_i(t + \Delta t) + \phi_i(t - \Delta t) - 2\phi_i(t)]/(\Delta t)^2$. Starting from an initial configuration, we update the equations of motion up to a certain maximum time $t_{\max}$. Then we repeat the procedure with other initial configurations. Reasonable results in two dimensions are obtained mainly with $\Delta t = 0.05$ up to $t_{\max} = 640$ and a lattice size $L = 521$ [11]. 200 samples of initial configurations are used for averaging. For three dimensions, we also perform the computations with $\Delta t = 0.05$ up to $t_{\max} = 640$ but with a lattice size $L = 125$. Here, 50 samples are taken for averaging. We have also carried out some computations with other Δt's and lattice sizes to confirm the results. At the time $t_{\max}$, the equal-time correlation function $C(r,t)$ decays to nearly zero at $r \sim 45$ and this indicates that the finite-size effect with $L = 128$ is already small. Furthermore, in order to gain more confidence in our conclusions, especially whether our $t_{\max}$ has really reached the scaling regime, we perform more accurate computations in two dimensions (compared with those in Ref. [11]) with a lattice size $L = 256$ and $\Delta t = 0.02$, 0.01 up to $t_{\max} = 1280$. The number of samples for averaging is 600. In this article, somewhat different and more careful approaches will be adopted.

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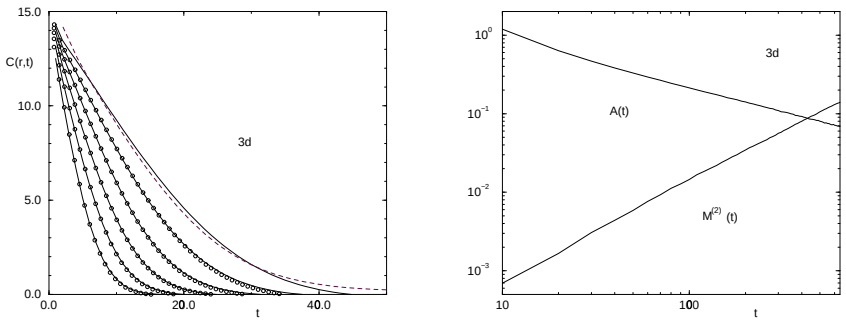

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Figure 2. a) $C(r,t)$ in three dimensions obtained with $L = 128$ and $\Delta t = 0.05$ is plotted with solid lines for $t = 20$, 40, 80, 160, 320, and 640 (from left). Circles fitted to the curve at the time t display the data at the time $2t$ with r being rescaled by a factor $2^{-1/z}$. The dashed line represents the scaling function in two dimensions. (b) $A(t)$ and $M^{(2)}(t)$ on a log-log scale.

In Fig. 1(a), the equal-time correlation function $C(r,t)$ in two dimensions is displayed. Solid lines are obtained with $\Delta t = 0.01$ and, from left to right, the time t is 20, 40, 80, 160, 320, 640, and 1280. Data for $\Delta t = 0.02$ are also plotted with dashed lines, but they almost completely overlap with the solid lines. For the curve of $t = 1280$, $C(r,t)$ decays to nearly zero at $r \sim 50$. Therefore, we conclude that the finite-size effect for the lattice size $L = 256$ should already be negligibly small. To confirm this, we have also compared the data with those in Ref. [11]. Our data also show that the finite Δt effect for $\Delta t = 0.05$ is negligible, too. According to the scaling form (6), from data collapse of $C(r,t)$ at different t's, one can estimate the dynamic exponent z. As observed in Ref. [11], the effective dynamic exponent $z(t)$ shows a small dependence on the time t. To explore this behavior and extract confidently the value of z, we perform scaling collapse of $C(r,t)$ with the time t and $2t$. In Fig. 1(a), circles fitted to a solid line of the time t are the data of the time $2t$ with r being rescaled by a factor $2^{-1/z}$, i.e. $C(r,t) = C(r2^{1/z}, 2t)$. The dynamic exponent $z(t)$ is determined by the best fitting of the circles to the corresponding solid line. We see clearly that the data collapse nicely.

Figure 2(a) shows $C(r,t)$ in three dimensions. Scaling collapse is also observed, even though for larger r it is not as good as in two dimensions. This can be neither a finite-size effect nor a finite Δt effect, since it exists also for small t's. To see the trend of $z(t)$ as the time t evolves, we plot in

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Fig. 3(a) the effective exponent $z(t)$ against $1/t$. For two dimensions, $z(t)$ starting from a value around 3 gradually *decreases* and reaches 2.63(2) at $t = 640$ (i.e. obtained with data of $C(r,t)$ at the time $t = 640$ and $2t = 1280$). Assuming that the behavior of $z(t)$ will not change essentially after $t = 1280$, the extrapolated value of z to the infinite time t is estimated to be 2.6(1). Interestingly, for three dimensions the exponent $z(t)$ starting from a value around 2.5 *increases* slowly, but stabilizes at 2.7 after $t = 80$. A good estimate of z is $z = 2.7(1)$. Within statistical errors, the values of the dynamic exponent z in two and three dimensions coincide with each other, thus indicating that the dynamic exponent z is dimension-independent. This can also be seen from the joining of two different curves at relatively large times in Fig. 3(a).

In the case of the Ising model with Monte Carlo dynamics, the effective exponent $z(t)$ in two dimensions converges to $z = 2$ rather fast (see Ref. [15]), but it is relatively slow in three dimensions due to corrections to scaling. It might be somewhat general that phase ordering dynamics in three dimensions is somewhat more complicated than in two dimensions.

An interesting fact is that even though the dynamic exponent z of the ϕ^4-theory in two dimensions with Hamiltonian dynamics is different from that of the Ising model with Monte Carlo dynamics, the scaling function $f(x)$ in Eq. (6) is the same [11]. However, this is probably only by chance since it is *not* the case in three dimensions. The scaling function $f(x)$ of the three-dimensional ϕ^4-theory with Hamiltonian dynamics is different not only from that of the two-dimensional but also from that of the three-dimensional Ising model with Monte Carlo dynamics. The dashed line in Fig. 2(a) shows the $f(x)$ of the two-dimensional ϕ^4-theory. In general, Hamiltonian dynamics for isolated systems differs indeed from stochastic dynamics for non-isolated systems.

For a simple understanding of the correlation function $C(r,t)$, one can measure the time-dependent second moment $M^{(2)}(t)$. The scaling form results in a power-law behavior for $M^{(2)}(t)$ and from the slope in log-log scale one can estimate the corresponding exponent. Such an approach is rather typical and useful in critical dynamics [14]. It can also be applied in ordering dynamics, but this is less efficient. In critical dynamics, in the scaling collapse of $C(r,t)$, one has to determine two exponents, the dynamic exponent z and the static exponent $2\beta/\nu$. Therefore it is efficient to read out directly the exponent $(d - 2\beta/\nu)/z$ from the slope of $M^{(2)}(t)$ in log-log scale [14].

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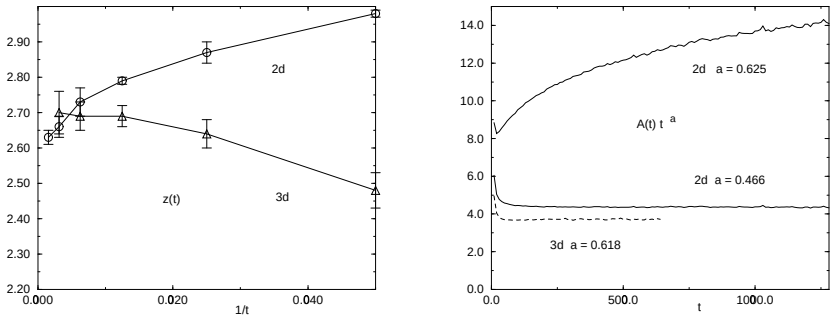

(*a*) (*b*)

Figure 3. (a) The effective dynamic exponent $z(t)$ measured from scaling collapse of $C(r,t)$ with the times t and $2t$. (b) Taking $a = \lambda/z$, $A(t)t^a$ tends to a constant.

However, in ordering dynamics the "static" exponent $2\beta/\nu = 0$ and the scaling collapse of $C(r,t)$ is only a one parameter fit. Measurements of $M^{(2)}(t)$ do not show any advantage since it is not self-averaged and there is a larger fluctuation for bigger lattices (see the data in Ref. [11]). Anyway, in Fig. 2(b) we have plotted the second moment in log-log scale for the three-dimensional ϕ^4-theory. The power-law behavior is seen after $t \sim 80$ and this is consistent with Fig. 3(a). According to Eq. (7), the resulting dynamic exponent is $z = 2.5(2)$, consistent within errors with $z = 2.7(1)$ measured from $C(r,t)$.

Another interesting exponent in ordering dynamics is λ governing the power-law decay of the auto-correlation $A(t)$ in Eq. (9). The measurements of the auto-correlation in ordering dynamics is easier than in critical dynamics since the fluctuation is much smaller. The results for the ϕ^4-theory in two and three dimensions are shown in Fig. 1(b) and 2(b). In order to see how the effective exponent λ/z depends on the time t, we have measured the slope of the curves in the time interval $[t, 2t]$. The results are given in Table 1. For both, two and three dimensions, the exponent λ/z becomes stable after $t = 160$. The final values are $\lambda/z = 0.466(3)$ and $0.618(4)$ for two and three dimensions, respectively. To show that our estimates of λ/z are indeed reasonable, we plot $A(t)t^a$ in Fig. 3(b) as a function of the time t. A correct value $a = \lambda/z$ should result in a constant for $A(t)t^a$, at least for larger times. Such a behavior is nicely seen from the lower solid line and the dashed line for two and three dimensions. To confirm that the value $\lambda/z = 0.466(3)$ for two dimensions is really different from $\lambda/z = 0.625$ for stochastic dynamics, the corresponding curve with $a = 0.625$ is also displayed there (the upper

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Table 1. The exponent λ/z measured in the time interval $[t, 2t]$ from the auto-correlations in two and three dimensions.

t	40	80	160	320	640
$2D$	0.508(1)	0.492(1)	0.469(7)	0.461(6)	0.463(6)
$3D$	0.633(4)	0.609(1)	0.617(3)	0.619(7)	

solid line). Obviously, it does not tend to a constant.

From measurements of z (from $C(r,t)$) and λ/z, we estimate the exponent $\lambda = 1.21(5)$ and $1.67(6)$ for two and three dimensions, respectively. For stochastic dynamics, the theoretical prediction for two dimensions is $\lambda = 1.25$ [12,16], but in Monte Carlo simulations it is usually slightly smaller [15]. Extrapolation is needed to obtain a value very close to 1.25. There is always some uncertainty in extrapolation. Therefore, we tend to claim that λ of the ϕ^4-theory in two dimensions with Hamiltonian dynamics is the same as that of stochastic dynamics. In three dimensions, our $\lambda = 1.67(6)$ agrees very well with the "best" theoretical prediction 1.67 for stochastic dynamics [12,17]. Numerical measurements of λ for stochastic dynamics in three dimensions look somewhat problematic and the results fluctuate around the theoretical values.

To complete our investigation, we have also simulated the initial increase of the magnetization in Eq. (10). Since the exponent θ is relatively big, compared with that in critical dynamics [11,14], we need to prepare a very small initial magnetization m_0.

In Fig. 4, the magnetization in three dimensions is plotted on a log-log scale for $m_0 = 0.00123$, 0.00245, and 0.00491 (from below), respectively. The power-law behavior is observed after $t \sim 50$. From the slope, we measure the exponent θ. Within statistical errors, we cannot find any m_0 dependence of θ. The value of θ is estimated to be 0.55(2). With θ in hand, combining $\lambda/z = 0.618(4)$, we obtain another value for the dynamic exponent, $z = 2.6(1)$.

In Table 2, all exponents measured for the ϕ^4-theory with Hamiltonian dynamics are summarized. Results for two dimensions are taken from Ref. [11], but λ/z, λ and z from $C(r,t)$ are slightly modified. Different measurements in two and three dimensions suggest that $z = 2.6(1)$ is a good estimate for the dynamic exponent. Since the critical exponent θ in phase ordering dynamics is different from the case of critical dynamics [14], it has not yet got enough attention, even though it has been mentioned in Ref. [12]. One reason might

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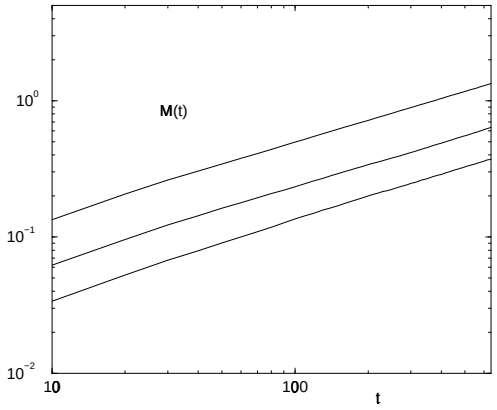

Figure 4. The magnetization in three dimensions on a log-log scale. The lattice size is $L = 128$. From below, $m_0 = 0.00123$, 0.00245, and 0.00491.

be that, in ordering dynamics!, increasing of the magnetization is expected if a non-zero initial value m_0 is set, but in critical dynamics, this is anomalous. Anyway, we think θ is interesting since it gives another independent estimate for the dynamic exponent z or λ.

4 Conclusions

We have numerically solved the Hamiltonian equations of motion for the two- and three-dimensional ϕ^4-theory with random initial states. Phase ordering dynamics is carefully investigated. Scaling behavior is confirmed. The dynamic exponent z is dimension-independent. Different measurements yield a value $z = 2.6(1)$ which differs from $z = 2$ for stochastic dynamics of model A. The scaling function for the equal-time spatial correlation function is dimension-dependent, and in general it is also different from that of stochastic dynamics of model A (this is the same probably only by chance in two dimensions). However, the exponent λ of Hamiltonian dynamics is the same as that of stochastic dynamics of model A.

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Table 2. Exponents of the ϕ^4-theory with Hamiltonian dynamics. To calculate λ, z measured from $C(r,t)$ is taken as input.

			z			
	θ	λ/z	$d/(\lambda/z+\theta)$	$C(r,t)$	$M^{(2)}$	λ
2D	0.31(1)	0.466(3)	2.6(1)	2.6(1)	2.6(1)	1.21(5)
3D	0.55(2)	0.618(4)	2.6(1)	2.7(1)	2.5(2)	1.67(6)

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