Deterministic equations of motion and phase ordering dynamics

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We numerically solve microscopic deterministic equations of motion for the two-dimensional ϕ^4 theory with random initial states. Phase ordering dynamics is investigated. Dynamic scaling is found and it is dominated by a fixed point corresponding to the minimum energy of random initial states.

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In recent years microscopic deterministic equations of motion (e.g., Newton, Hamiltonian and Heisenberg equations) have attracted much attention of scientists in different areas. From fundamental view points, solutions of deterministic equations may describe both equilibrium and nonequilibrium properties of statistical systems, even though a general proof does not exist, e.g., see Refs. [1–5]. Ensemble theories and stochastic equations of motion are effective descriptions of static and dynamic properties of the statistical systems, respectively. With recent development of computers, it becomes possible to solve deterministic equations numerically. For example, recently attempt has been made for the O(N) vector model and XY model [5–7]. The results support that deterministic equations correctly describe second order phase transitions. The estimated static critical exponents are consistent with those calculated from canonical ensembles. More interestingly, the macroscopic short-time (nonequilibrium) dynamic behavior of the two-dimensional (2D) ϕ^4 theory at *criticality* has also been investigated and dynamic scaling is found [8,9]. The results indicate that deterministic dynamics with random initial states is in a same universality class of Monte Carlo dynamics of model A.

On the other hand, phase ordering dynamics has been investigated for years [10]. It concerns how a statistical system evolves into an ordered phase after a quench from a disordered phase. For example, the Ising model initially at a very high temperature T_I is suddenly quenched to a temperature T_F well below the critical temperature T_C, and then evolves dynamically. Because of the competition of the two ordered phases, it is well known that the equilibration is very slow. Investigation reveals that in the *late* stage (in microscopic sense) of the dynamic evolution there emerges scaling behavior, which is somehow universal. The scaling behavior is dominated by the fixed point $(T_I,T_F)=(\infty,0)$ and away from the fixed point there are corrections to scaling.

Up to now, for simple systems *stochastic* dynamics described by Langevin-type equations or Monte Carlo algorithms has been studied. Scaling behavior of ordering dynamics depends essentially on whether the order parameter is conserved (model B) or not (model A). For the Ising model (or ϕ^4 theory), the dynamic exponent is $z=2$ for model A and $z=3$ for model B [10].

The purpose of this paper is to study the phase ordering dynamics with the microscopic deterministic equations of motion, taking the 2D ϕ^4 theory as an example.

Following Refs. [8,5] we consider an isolated system. The Hamiltonian of the 2D ϕ^4 theory on a square 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 $\pi_i=\dot{\phi}_i$ and it leads to the equations of motion

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

Energy is conserved in these equations. Solutions in the long-time regime are assumed to generate a microcanonical ensemble. The temperature could be defined as the averaged kinetic energy. For the dynamic system, however, the total energy is an even more convenient controlling parameter of the system, since it is conserved and can be 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 disordered phase (above ϵ_c). The phase transition is of the second order.

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

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

The average is *over initial configurations* and L is the lattice size.

Following ordering dynamics with stochastic equations, we consider a dynamic process that the system initially in a *disordered* state but with energy density well below ϵ_c is suddenly released to evolve according to Eq. (2). For simplicity, we set 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 unit of c, and finally the constant c is determined by the given energy. We could also give a distribution for $|\phi_i(0)|$ but the difference will only be corrections to scaling.

In the case of stochastic dynamics, scaling behavior of phase ordering is dominated by the fixed point $(T_I,T_F)=(\infty,0)$. In deterministic dynamics, 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

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

Here d is the spatial dimension. The conjecture is that the scaling behavior is dominated by the minimum energy density $v_{\min}=V_{\min}/L^2$, which is a kind of fixed points. In this paper, we consider the case of $d<m^2/2$. Then $v_{\min}=-6(d-m^2/2)^2/g$. From now, we redefine the energy density $e_{\min}$ as zero. Then the fixed point is $\epsilon_0=v_{\min}-e_{\min}$.

To solve the equations of motion (2) numerically, we discretize $\ddot{\phi}_i$ by $[\phi_i(t+\Delta t)+\phi_i(t-\Delta t)-2\phi_i(t)]/(\Delta t)^2$. After an initial configuration is prepared, we update the equations of motion until $t=650$ or 1000. Then we repeat the procedure with other initial configurations. From the experience in Refs. [8,9], $\Delta t=0.05$ is small enough for our updating times. In our calculations, we use mainly a lattice size $L=512$ and samples of initial configurations for average are 200. Some simulations have also been performed for $L=1024$ with 50 samples to estimate the finite size effect.

An important observable is the equal-time correlation function

$$C(r,t)=\frac{1}{L^2}\left\langle \sum_i \phi_i(t)\phi_{i+r}(t)\right\rangle. \tag{5}$$

Here the lattice site $i+r$ is away from i with a distance r. The scaling hypothesis is that at the late stage of the time evolution, $C(r,t)$ obeys a scaling form

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

where z is the so-called dynamic exponent and the initial magnetization $m_0=0$. For stochastic dynamics, this scaling form is valid for all temperatures well below the critical temperature. Monte Carlo simulations, e.g., for the Ising model, actually show that at the fixed point $(T_I,T_F)=(\infty,0)$ the scaling behavior often emerges at a relatively early time t in the *macroscopic* sense [11,12], after a time scale $t_{\rm mic}$ which is large enough in the microscopic sense. Away from the fixed point, there are corrections to scaling. For deterministic dynamics, we expect that the minimum energy density of the random initial states $\epsilon_0=v_{\min}-e_{\min}$ plays a similar role.

Another interesting observable is the autocorrelation function

$$A(t)=\frac{1}{L^2}\left\langle \sum_i \phi_i(0)\phi_i(t)\right\rangle. \tag{7}$$

The scaling hypothesis for the autocorrelation $A(t)$ is a power law behavior

$$A(t)\sim t^{-\lambda/z}. \tag{8}$$

It implies a divergent correlation time and ordering dynamics is in some sense ''*critical.*'' Here λ is another independent exponent.

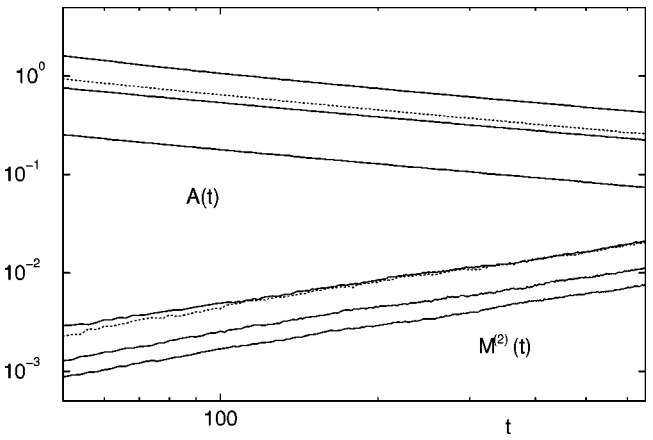

FIG. 1. The autocorrelation and the second moment with $L=512$ plotted in log-log scale. Solid lines for $A(t)$ are for $(m^2,g)=(8.0,2.4)$, $(6.0,1.8)$, and $(6.0,5.4)$ (from above) at the fixed points, while for $M^{(2)}(t)$ are for $(m^2,g)=(6.0,1.8)$, $(8.0,2.4)$, and $(6.0,5.4)$ (from above). Dashed lines correspond to $(m^2,g)=(6.0,1.8)$ but energy density is 4/3 above the fixed point.

We have carried out computations with a lattice size $L=512$ for parameters $(m^2,g)=(6.0,1.8)$, $(6.0,5.4)$, and $(8.0,2.4)$ at the fixed point ϵ_0. For $(m^2,g)=(6.0,1.8)$, extra simulations with energy density $\epsilon=\epsilon_0+4/3$ and at ϵ_0 with a large lattice $L=1024$ have been performed. The autocorrelation has been plotted in Fig. 1. The curve for $(m^2,g)=(6.0,1.8)$ with $L=1024$ (not in the figure) overlaps with that for $L=512$. In the figure, we see clearly a nice power law behavior after $t_{\rm mic}\sim 50-100$. The dashed line is for $(m^2,g)=(6.0,1.8)$ with energy density $\epsilon=\epsilon_0+4/3$ and correction to scaling is still not so big. All curves having nearly the same slope indicate a kind of universality and the fixed point plays an important role. As is the case of the Ising model with Monte Carlo dynamics [11], there is a small curvature in the curves, but upwards. This gives rise to about one or two percent difference of the slope depending on the measured time interval. Slopes for different curves have also a comparable uncertainty. Taking into account all these factors and statistical errors, we estimate the exponent $\lambda/z=0.460(10)$.

In Fig. 2, the equal-time correlation function $C(r,t)$ is displayed. The curves are for $(m^2,g)=(6.0,1.8)$ with $L=1024$ and one sees clear self-similarity during time evolution. According to the scaling form (6), data for different time t should collapse if r is suitably rescaled by $t^{1/z}$. In other words, searching for the best collapse of the data we can obtain the dynamic exponent z. This collapse of the data is shown on the first curve from the left. All data points locate nicely on a curve except for a small departure for $t=20$. The corresponding dynamic exponent measured from a time interval $[40,640]$ is $z=2.69(9)$. In Table I, we list values of z for different parameters and measured in different time intervals. Again, for larger time t the dynamic exponent z tends to be slightly smaller. We believe the small deviation for different parameters (m^2,g) is more or less due to uncontrolled systematic errors or/and possible corrections to scaling. From the table, we estimate the dynamic exponent $z=2.65(10)$. This is significantly different from $z=2.0$ for the Ising model with stochastic dynamics of model A.

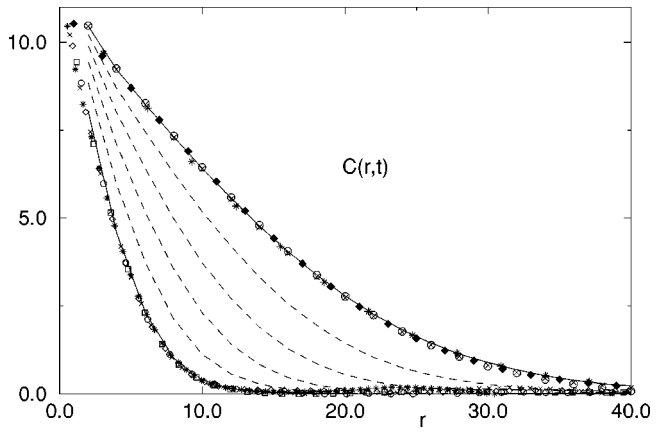

FIG. 2. Scaling plot for $C(r,t)$. Six curves for $(m^2,g)=(6.0,1.8)$ at fixed point with $L=1024$ correspond $t=20$, 40, 80, 160, 320, and 640 (from left). ○, □, ◇, ×, and * fitted to the curve of $t=20$ are those for $t=40$ to 640 but r is rescaled according to $r/t^{1/z}$ with $z=2.69$. × and * fitted to the curve of $t=640$ are data for $(m^2,g)=(6.0,5.4)$ and $(8.0,2.4)$ at the fixed points and ○ for $(m^2,g)=(6.0,1.8)$ with energy density 4/3 above the fixed point. The lattice size is $L=512$ and both axes are rescaled with suitable constants. Full diamonds represent the scaling function for the Ising model at the zero temperature.

Very interesting is that the scaling function $f(x)$ in Eq. (6) for the ϕ^4 theory is the same as that of the Ising model with Monte Carlo dynamics of model A [11,13], even though the exponent z is different. This is shown on the last curve from left in Fig. 2. To plot the functions, r and $C(r,t)$ have been suitably rescaled by constants. We did not try to get a ''best'' fit to all the data but only to show they are indeed a same function. For the data of $(m^2,g)=(6.0,5.4)$ (×) and (6.0,5.4) (○), only r is rescaled. For the Ising model (full diamonds), the rescaling factor for r happens to be 1/2.

A 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 a power law behavior

$$M^{(2)}(t)\sim t^{d/z}. \tag{9}$$

This is shown also in Fig. 1. Even though there are some visible fluctuations, power law behavior is observed. From slopes of the curves after $t\sim 100$, we measure the exponent $d/z=0.76(3)$. Then we estimate the dynamic exponent $z=2.63(10)$.

For discussions above, the initial magnetization m_0 is zero. If m_0 is a nonzero, the system reaches a unique ordered state within a finite time. If m_0 is infinitesimal 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 macroscopic sense). In this case, an interesting observable is the magnetization itself and at early times 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 deeply been investigated in critical dynamics [14,15].

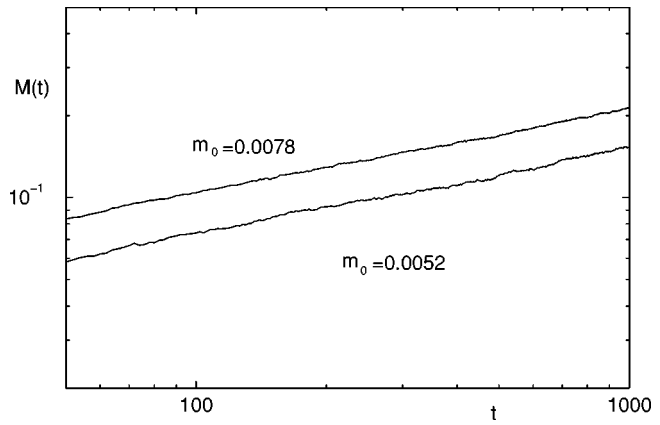

FIG. 3. The magnetization in log-log scale. The lattice size is $L=512$.

In Fig. 3, the initial increase of the magnetization is shown. After $t_{\rm mic}\sim 80$, nice power law behavior is seen. To avoid finite m_0 effect, very small values of m_0 have been chosen. The resulting exponent θ is 0.308(9) and 0.315(30) for $m_0=0.0078$ and 0.0052, respectively. Taking into account the errors, we consider $\theta=0.308(9)$ as the final result. With θ and λ/z in hand, from the scaling relation $\theta=(d-\lambda)/z$ again we can calculate the dynamic exponent $z=2.60(5)$.

In Table II, we have summarized all the measurements of the exponents. The agreement of different measurements of z strongly supports the dynamic scaling hypothesis. The exponents of the Ising model with stochastic dynamics of model A are from theoretical calculations [12,10]. In Monte Carlo simulations, there may be small deviation [12,16,11]. It is interesting that the dynamic exponent z for the ϕ^4 theory with deterministic dynamics is clearly different from that of the Ising model with stochastic dynamics but the exponent λ looks the same.

In Refs. [8,9,15], we know that in dynamic critical phenomena, deterministic dynamics for the 2D ϕ^4 theory and

TABLE I. The dynamic exponent z estimated from scaling collapse of $C(r,t)$ in a time interval $[t_1,640]$. If not specified, the lattice size $L=512$ and the energy density is at its fixed points.

(m^2,g)		$t_1=40$	$t_1=80$	$t_1=160$	$t_1=320$
(8.0,2.4)		2.84(5)	2.83(6)	2.76(10)	2.79(12)
(6.0,5.4)		2.75(2)	2.75(1)	2.70(1)	2.72(1)
(6.0,1.8)		2.78(3)	2.76(1)	2.67(3)	2.57(4)
	$L=1024$	2.72(7)	2.69(9)	2.67(7)	2.66(4)
	$\epsilon=\epsilon_0+4/3$	2.78(5)	2.74(8)	2.70(10)	2.69(10)

TABLE II. Exponents of the ϕ^4 with deterministic dynamics. To calculate λ, z measured from $C(r,t)$ is taken as input. Values for the Ising model are theoretical results with stochastic dynamics of model A [12,10].

			z			
	θ	λ/z	$d/(\lambda/z+\theta)$	$C(r,t)$	$M^{(2)}$	λ
ϕ^4	0.308(9)	0.460(10)	2.60(5)	2.65(10)	2.62(10)	1.22(5)
Ising		0.625		2		1.25

stochastic dynamics of model A for the Ising model are in a same universality class. Why is it not the case in ordering dynamics? This may be traced back to the energy conservation in our deterministic equations. Since energy couples to the order parameter, deterministic dynamics is somehow believed to be a realization of model C [17]. For critical dynamics, in two dimensions model A and model C are the same. For ordering dynamics, however, model A and model C can be different. It is pointed out in Ref. [17] that in many cases real physical systems may be intermediate between model A and C.

When $d-m^2/2$ becomes positive, $v_{\min}$ moves to zero. This is an unnormal fixed point $[\phi_i(0)\equiv 0]$, from which the system cannot move. Around this fixed point, self-similarity is also observed in time evolution, but a simple scaling form as Eq. (6) does not give good collapse of the data, at least up to the time $t=650$. Further understanding remains open.

In conclusion, we have investigated ordering dynamics governed by deterministic equations of motion, taking the 2D ϕ^4 theory as an example. Scaling behavior is found and it is dominated by the fixed point corresponding to the minimum energy of random initial states. The dynamic exponent z is different from that of stochastic dynamics of model A, while the scaling function for the equal-time correlation $C(r,t)$ is the same. Deterministic dynamics with energy conservation might be a realization of model C.

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