Microscopic Deterministic Dynamics and Persistence Exponent

B. Zheng

FB Physik, Universität – Halle, 06099 Halle, Germany

Abstract

Numerically we solve the microscopic deterministic equations of motion with random initial states for the two-dimensional $\phi^4$ theory. Scaling behavior of the persistence probability at criticality is systematically investigated and the persistence exponent is estimated.

PACS: 64.60.Ht, 11.10.-z
Recently the persistence exponent has attracted much attention. This exponent was first introduced in the context of the non-equilibrium coarsening dynamics at zero temperature \cite{1,2}. It characterizes the power law decay of the persistence probability that a local order parameter keeps its sign during a time \( t \) after a quench from a very high temperature to zero temperature. For critical dynamics, the local order parameter (usually, a spin) flips rapidly and the persistence probability does not obey a power law. In this case, however, the persistence exponent \( \theta_p \) can be defined by the power law decay of the global persistence probability \( p(t) \) that the global order parameter has not changed the sign in a time \( t \) after the quench from a very high temperature to the critical temperature \cite{3},

\[
p(t) \sim t^{\theta_p}.
\]

An interesting property of the persistence exponent is that its value is highly non-trivial even for simple systems. For the quench to zero temperature, for example, \( \theta_p \) is apparently not a simple fraction for the simple diffusion equation and the Potts model in one dimension \cite{4,5}. For the quench to the critical temperature, it is shown that the persistence exponent is generally a new independent critical exponent, i.e. it can not be expressed by the known static exponents, the dynamic exponent \( z \) and the recently discovered exponent \( \theta \) \cite{3,6}. This relies on the fact that the time evolution of the global magnetization is not a Markovian process. Recent Monte Carlo simulations for the Ising and Potts model at criticality support the power law decay of the global persistence probability and detect also the non-Markovian effect \cite{7,8}.

Up to now, the persistence exponent has been studied only in stochastic dynamic systems, described typically by Langevin equations or Monte Carlo algorithms. From fundamental view points, both equilibrium and non-equilibrium properties of statistical systems can be described by the microscopic deterministic equations of motion (e.g. Newton, Hamiltonian and Heisenberg equations) \footnote{Langevin equations at zero temperature are also deterministic, but they are at mesoscopic level and generally different from the microscopic deterministic equations of motion.} even though a general proof does not exist. With recent development of computers, gradually it becomes possible to solve numerically the microscopic deterministic equations of motion. For example, the \( O(N) \) vector model and the \( XY \) model have been investigated \cite{9–11}. The results confirm that the deterministic equations describe correctly second order phase transitions. The static critical exponents are estimated and agree with existing values. More interestingly, in a recent paper short-time dynamic behavior of the deterministic dynamics starting from random initial states has been studied \cite{12}. The short-time dynamic scaling was found and the estimated value of the dynamic exponent \( z \) is the same as that of the Monte Carlo dynamics of the Ising model.

The purpose of this letter is to study the critical scaling behavior of the global persistence probability and measure the persistence exponent in microscopic deterministic dynamic systems, taking the two-dimensional \( \phi^4 \) theory as an example.

The Hamiltonian of the two-dimensional \( \phi^4 \) theory on a square lattice is written as

\[
H = \sum_i \left[ \frac{1}{2} \pi_i^2 + \frac{1}{2} \sum_\mu (\phi_{i+\mu} - \phi_i)^2 - \frac{1}{2} m^2 \phi_i^2 + \frac{1}{4!} \lambda \phi_i^4 \right].
\]
with \( \pi_i = \dot{\phi}_i \) and it leads to the equations of motion

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

Energy is conserved during the dynamic evolution governed by Eq. (3). As discussed in Refs. [9,12], a microcanonical ensemble is assumed to be generated by the solutions. In this case, the temperature could not be introduced externally as in a canonical ensemble, but could only be defined internally as the averaged kinetic energy. In the dynamic approach, the total energy is actually an even more convenient controlling parameter of the system, since it is conserved and can be input from the initial state.

From the viewpoint of ergodicity, to achieve a correct equilibrium state the microscopic deterministic dynamic system should start from a random initial state. Interestingly, this is just similar to the dynamic relaxation in stochastic dynamics after a quench from a very high temperature. Therefore, similar dynamic behavior may be expected for both dynamic systems.

The order parameter of the \( \phi^4 \) theory is the magnetization \( M(t) = \sum_i \phi_i(t)/L^2 \) with \( L \) being the lattice size. In this paper, we are interested in the global persistence probability \( p(t) \) at the critical point, which is defined as the probability that the not averaged order parameter has not changed the sign in a time \( t \) starting from a random state with small initial magnetization \( m_0 \).

Following Ref. [12], we take parameters \( m^2 = 2 \) and \( \lambda = 0.6 \) and prepare the initial configurations as follows. For simplicity, we set initial kinetic energy to be zero, i.e. \( \dot{\phi}_i(0) = 0 \). We fix the magnitude of the initial field to be a constant \( c \), \( |\phi_i(0)| = c \), and 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.

To solve the equations of motion (3) numerically, we simply discretize \( \ddot{\phi}_i \) by \( (\phi_i(t + \Delta t) + \phi_i(t - \Delta t) - 2\phi_i(t))/\Delta t^2 \). According to the experience in Ref. [12], \( \Delta t \) is taken to be 0.05. After an initial configuration is prepared, we update the equations of motion until the magnetization changes its sign. The maximum observing time is \( t = 1000 \). Then we repeat the procedure with other initial configurations and measure the persistence probability \( p(t) \). In our calculations, we use fairly large lattices \( L = 128 \) and 256 and samples of initial configurations range from 3 500 to 30 000 depending on initial magnetization \( m_0 \) and lattice sizes. The smaller \( m_0 \) and lattice size \( L \) are, the more samples of initial configurations we have. Errors are simply estimated by dividing total samples into two or three subsamples. Compared with Monte Carlo simulations, our calculations here are much more time consuming due to the small \( \Delta t \).

According to analytical analyses and Monte Carlo simulations in stochastic dynamic systems, at the critical point and in the limit \( m_0 = 0 \), \( p(t) \) should decay by a power law as in Eq. (4). Our first effort is to investigate whether in microscopic deterministic dynamics \( p(t) \) obeys also the power law and measure the persistence exponent \( \theta_p \).

Here we adopt the critical energy density \( \epsilon_c = 21.1 \) from the literature [1,2]. In Fig. 4, the persistence probability \( p(t) \) is displayed on a log-log scale for lattice sizes \( L = 256 \) and 128 with solid lines and a dash line respectively. For \( L = 256 \) simulations have been performed with two values of initial magnetization \( m_0 = 0.003 \) and 0.0015. These straight lines convince us the power law behavior of \( p(t) \). Skipping data within a microscopic time scale \( t \sim 100 , \)
from the slopes of the curves one estimates the persistence exponent $\theta_p = 0.252(6)$ for both values of $m_0$. This shows that there is already no effect of finite $m_0$. The curve for $L = 128$ and $m_0 = 0.0015$ is roughly parallel to that of $L = 256$. One measures the the slope $\theta_p = 0.251(1)$ in the time interval $[100, 500]$ but $\theta_p = 0.232(10)$ in $[100, 1000]$. This indicates that some finite size effect exists still for $L = 128$ after $t = 500$ but is negligible small for $L = 256$.

If the time evolution of the magnetization is a Markovian process, from theoretical view points the persistence exponent will be not an independent critical exponent and it will take the value $\alpha_p$, which relates to other exponents through

$$\alpha_p = -\theta + (d/2 - \beta/\nu)/z.$$  \hfill (4)

In Table I, values of the exponent $\theta_p$, $z$, $\theta$ and $\alpha_p$ for the $\phi^4$ theory are given in comparison with those of the kinetic Ising model induced by local Monte Carlo algorithms. As is the case of the Ising model, the exponents $\theta_p$ and $\alpha_p$ for the $\phi^4$ theory differ also by about 10 percent. This represents a rather visible non-Markovian effect in the time evolution of the magnetization.

For equilibrium states, it is generally believed that the $\phi^4$ theory and the Ising model are in a same universality class. Results from numerical solutions of the deterministic equations also support this. From the short-time dynamic approach, within statistical errors the dynamic exponent $z$ for the microscopic deterministic dynamics of the $\phi^4$ theory is the same as that of the kinetic Ising model with Monte Carlo algorithms but the exponent $\theta$ differs by several percent. In Table I, we see that $\theta_p$ for the $\phi^4$ theory is also several percent bigger than that of the Ising model. However, by feeling we still think that the $\phi^4$ theory and the Ising model are very probably in a same persistence universality class. These same percent differences of the exponents come probably from that the critical point $\epsilon_c$ has not been very accurate or there are some corrections to scaling and uncontrolled systematic errors. Actually, we will see below that the critical energy density could be somewhat lower than $\epsilon_c = 21.1$ and it would yield a slightly smaller $\theta_p$.

Our second step is to investigate the scaling behavior of the persistence probability in the neighborhood of the critical energy density. From general view points of physics, one may expect a following scaling form

$$p(t, \tau) = t^{-\theta_p} F(t^{1/\nu z} \tau).$$  \hfill (5)

Here $\tau = (\epsilon - \epsilon_c)/\epsilon_c$ is the reduced energy density. When $\tau = 0$, the power law behavior in Eq. (4) is recovered. When $\tau$ differs from zero, the power law will be modified by the scaling function $F(t^{1/\nu z} \tau)$. In principle, this fact may be used for the determination of the critical energy density. In Fig. 2, $p(t, \tau)$ for $L = 256$ and $m_0 = 0.003$ is plotted for three different energy density $\epsilon = 20.9, 21.1$ and 21.3. In the figure, we see that the solid line shows the

---

2In deterministic dynamics, energy is conserved and it couples to the order parameter. Therefore, it is believed that the deterministic dynamics belongs to the dynamics of model C rather than model A. Standard local Monte Carlo dynamics of the Ising model is dynamics of model A. In two dimensions, model A and C are the same but maybe up to a logarithmic correction.
best power law behavior among the three curves. However, an very accurate estimate of $\epsilon_c$ could not be achieved so easily, since $p(t, \tau)$ is not so sensitive to the energy. According to our data, we estimate $\epsilon_c = 21.06(12)$. Within errors, it is consistent with $\epsilon_c = 21.1$ given in [4] and $\epsilon_c = 21.11(3)$ in [12]. We should point out, that the exponent $\theta_p$ will be 0.245, if it is measured at $\epsilon_c = 21.06$. It is closer to that of the kinetic Ising model, as discussed above.

In order to have more understanding of the scaling form [3], we differentiate with respect to the energy density on both sides of the equation and obtain

$$\partial_{\tau} \ln p(t, \tau) |_{\tau=0} \sim t^{1/\nu_z}.$$  

Using the data of Fig. 2, we can approximately calculate $\partial_{\tau} \ln p(t, \tau)|_{\tau=0}$ and the result is displayed in Fig. 3. Even though there are some fluctuations, power law behavior is still seen. The best fitted slope of the curve gives $1/\nu_z = 0.47(4)$ in the time interval [100, 1000]. Taking $z = 2.15(2)$ as input, one obtains $\nu = 0.99(8)$. Compared with $\nu = 1$ for the Ising model, this result supports that the $\phi^4$ theory with deterministic dynamics and the Ising model are in a same universality class.

Finally we study the scaling behavior of the persistence probability in case the initial magnetization is not so small and its effect can not be neglected. Following Ref. [8], we assume a finite size scaling form

$$p(t, L, m_0) = t^{-\theta_p} F(t^{1/z}L^{-1}, t^{x_{0p}/z}m_0).$$  

Here the energy density has been set to its critical value and $x_{0p}$ is the scaling dimension of the initial magnetization $m_0$. It was discovered that for the Ising model with Monte Carlo dynamics, the value $x_{0p} = 1.01(1)$ is ‘anomalous’, i.e. it is different from the scaling dimension of the initial magnetization $x_0 = 0.536(2)$ measured from the time evolution of the magnetization or auto-correlation [5]. The origin should be that $p(t, L, m_0)$ is a non-local observable in time $t$. It remembers the history of the time evolution.

To verify the scaling form [7] and estimate $x_{0p}$, we perform a simulation with the lattice size $L_1 = 256$ and initial magnetization $m_{01} = 0.0151$. Suppose the scaling form [3] holds, one can find an initial magnetization $m_{02}$ with the lattice size $L_2 = 128$ such that the curves of $p(t, L, m_0)$ for both lattice sizes collapse. Practically we have performed simulations for $L_2 = 128$ with two initial magnetizations, $m_0 = 0.0272$ and 0.0349. By linear extrapolation, we obtain data with $m_0$ between 0.0272 and 0.0349. Searching for a curve best fitted to the curve for $L_1 = 256$, we determine $m_{02}$. In Fig. 4, such a scaling plot is displayed. The lower and upper solid lines are the persistence probability for $L_2 = 128$ with $m_0 = 0.0272$ and 0.0349 respectively, while the dashed line is the properly rescaled one for $L_1 = 256$ with $m_{01} = 0.0151$. The solid line fitted to the dashed line represents the persistence probability for $L_2 = 128$ with $m_{02} = 0.0313(3)$. Since the microscopic time scale is $t_{mic} \sim 100$, nice collapse of the two curves can be observed only after $t \sim 100$. From the scaling form [7], $m_{02} = 2^{x_{0p}} m_{01}$ and one estimates $x_{0p} = 1.05(1)$. This value is very close to $x_{0p} = 1.01(1)$ for the kinetic Ising model.

In conclusions, we have numerically solved the microscopic deterministic equations of motion with random initial states for the two-dimensional $\phi^4$ theory and systematically investigated the critical scaling behavior of the persistence probability. As summarized in Table 4, the estimated exponents $\theta_p$ and $x_{0p}$ are very close to those of the kinetic Ising model induced by local Monte Carlo algorithms. What would be the dynamic and static behavior
of the deterministic dynamics starting from more general initial states is an interesting work in future.

Acknowledgements: Work supported in part by the Deutsche Forschungsgemeinschaft under the project TR 300/3-1.
REFERENCES

[1] B. Derrida, A.J. Bray and C. Godrèche, J. Phys. A27, L357 (1994).
[2] A. J. Bray, B. Derrida and C. Godrèche, Europhys. Lett. 27, 175 (1994).
[3] S.N. Majumdar, A.J. Bray, S. Cornell and C. Sire, Phys. Rev. Lett. 77, 3704 (1996).
[4] B. Derrida, V. Hakim and V. Pasquier, Phys. Rev. Lett. 75, 751 (1995).
[5] S.N. Majumdar, C. Sire, A.J. Bray and S. Cornell, Phys. Rev. Lett. 77, 2867 (1996).
[6] K. Oerding, S.J. Cornell and A.J. Bray, Phys. Rev. E56, R25 (1997).
[7] D. Stauffer, Int. J. Mod. Phys. C7, 753 (1996).
[8] L. Schülke and B. Zheng, Phys. Lett. A 233, 93 (1997).
[9] L. Caiani, L. Casetti and M. Pettini, J. Phys. A31, 3357 (1998).
[10] L. Caiani, L. Casetti, C. Clementi, G. Pettini, M. Pettini and R. Gatto, Phys. Rev. E57, 3886 (1998).
[11] X. Leoncini and A.D. Verga, Phys. Rev. E57, 6377 (1998).
[12] B. Zheng, M. Schulz and S. Trimper, Phy. Rev. Lett. 82, 1891 (1999).
[13] P.C. Hohenberg and B.I. Halperin, Rev. Mod. Phys. 49, 435 (1977).
[14] K. Oerding, private communication, 1999.
[15] B. Zheng, Int. J. Mod. Phys. B12, 1419 (1998), review article.
FIGS. 1-3

FIG. 1. The persistence probability is displayed in log-log scale for $\epsilon_c = 21.1$. Solid lines and a dashed line are for lattice sizes $L = 256$ and 128 respectively.

FIG. 2. The persistence probability is displayed in log-log scale for the energy densities $\epsilon = 20.9$, 21.1 and 21.3 (from above).

FIG. 3. The logarithmic derivative of the persistence probability with respect to the energy density is plotted in log-log scale, using the data in Fig. 2. The dashed line is the best fitted straight line.
FIG. 4. The scaling plot for the persistence probability. The lower and upper solid lines are the persistence probability for $L_2 = 128$ with $m_0 = 0.0272$ and 0.0349 respectively, while the dashed line is the properly rescaled one for $L_1 = 256$ with $m_{01} = 0.0151$. The solid line fitted to the dashed line represents the persistence probability for $L_2 = 128$ with $m_{02} = 0.0313(3)$. 
TABLE I. The critical exponents measured for the $\phi^4$ theory in comparison with those of the Ising model. The value of $\nu$ for the Ising model is exact, while others are taken from Table 2 in Ref. [15] and from Ref. [8]. $z$ and $\theta$ for the $\phi^4$ theory are from Ref. [12]. To calculate $\alpha_p$ for the $\phi^4$ theory $\beta/\nu = 1/8$ is taken as input.

|       | $\theta_p$ | $z$    | $\theta$ | $\alpha_p$ | $1/\nu z$ | $\nu$   | $x_{0p}$ |
|-------|------------|--------|----------|------------|-----------|---------|----------|
| $\phi^4$ | 0.252(6)  | 2.15(2)| 0.176(7) | 0.231(7)   | 0.47(4)   | 0.99(8) | 1.05(1)  |
| Ising  | 0.238(3)  | 2.155(3)| 0.191(1) | 0.215(1)   | 1         |         | 1.01(1)  |