Dynamic approach to weak first-order phase transitions

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A short-time dynamic approach to weak first-order phase transitions is proposed. Taking the two-dimensional Potts models as examples, from short-time behavior of nonequilibrium relaxational processes starting from high temperature and zero temperature states, pseudo-critical-points K^* and K^{**} are determined. A clear difference of the values for K^* and K^{**} distinguishes a weak first-order transition from a second-order one.

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In recent years, much progress has been achieved in nonequilibrium critical dynamics. For example, in a dynamic process in which a system initially at a high temperature or a zero temperature state is suddenly quenched to the critical temperature or nearby and then evolves dynamically, *short-time* universal scaling behavior has been found [1,2]. This phenomenon is rather fundamental. It exists not only in stochastic dynamics described by Langevin equations [1,3] or Monte Carlo algorithms [2,4–8], but also in deterministic dynamics described by fundamental microscopic equations of motion [9]. More interestingly, based on the short-time scaling form, it is possible to determine not only dynamic exponents but also static exponents as well as the *critical* temperature [10,11]. Since the measurements are carried out in the short-time regime, one does *not* suffer from critical slowing down. Compared with *nonlocal* cluster algorithms, the short-time dynamic approach does study properties of the local dynamics and applies to systems with quenched randomness. For a review, see Ref. [12].

Naturally, it is interesting and attractive to explore possible applications of short-time dynamics to *first*-order phase transitions. Especially, due to large correlation lengths and small discontinuities, a *weak* first-order transition presents quite similar behavior as a second-order one. It has long been challenging how to distinguish one from the other. Furthermore, *slowing down* in Monte Carlo simulations at first-order transitions is even more severe than at second-order ones. Nonlocal cluster algorithms also do not show much more efficiency.

In numerical simulations at first-order transitions *in equilibrium*, to locate the transition point one usually searches for the maximums of the specific heat, susceptibility, or a Binder cumulant constructed from energy [13]. For a system with lattice size L, these maximums deviate from the real transition point by a power law $1/L^d$. To remove this power law deviation, special techniques have been introduced [14]. With these techniques, first-order transition points can be determined rather accurately from moderate lattice sizes, even for weak first-order transitions.

To distinguish a first-order transition from a second-order one, naively one may explore a signal for discontinuity of the order parameter by increasing the lattice sizes. Refined methods are typically based on the *finite size scaling* of the specific heat, susceptibility, order parameter, Binder cumulant of energy, or the transition point, e.g., see Refs. [13,15–21]. However, when a first-order transition is very weak, it becomes subtle. The lattice sizes one reaches in simulations hardly feel the difference between very large correlation lengths in weak first-order transitions and divergent ones in second-order transitions. The double peak structure of the energy distribution together with the finite size scaling shows its merit in this respect [22–24], but further efficient methods are still desired.

In this Brief Report, we propose a short-time dynamic approach to weak first-order transitions. As examples, we investigate the two-dimensional q-state Potts models. The transition point is exactly known at $K_c=\ln(1+\sqrt{q})$. The phase transition is second order for $q\leqslant 4$ and becomes first-order for $q\geqslant 5$. For small q, the first-order transitions are weak. Especially, for $q=5$ the transition is so weak that with standard methods one hardly sees difference from a second-order one.

At a second-order transition point, short-time behavior of physical observables is a power law in dynamic processes starting from *both* a random and an ordered state. Away from the critical point, the power law behavior is modified by a scaling function [12]. At a first-order transition point, independent of initial states, physical observables do not present a power law behavior due to the finite correlation time or the symmetry breaking. If the transition point is known, this is already a signal for first-order transitions. If the transition point is not known, we need further investigations.

Around a first-order transition point, it is well known that for $K>K_c$ there is a *disordered metastable* state, which vanishes at a certain K^*. For $K<K_c$ there exists an *ordered metastable* state, which disappears at K^{**}. For a *weak* first-order transition, both K^* and K^{**} look like *critical* points if the system remains in the disordered and ordered metastable states, respectively. They are named *pseudo* critical points [25,26]. In equilibrium, numerical measurements of K^* and K^{**} are not easy due to finite-size effects. However, in short-time dynamics, K^* and K^{**} can be determined rather confidently. Starting from a high temperature state, for $K>K_c$ the system reaches the disordered metastable state first. Due to the large correlation time induced by the large spatial correlation length in the metastable state, at K^* physical ob-

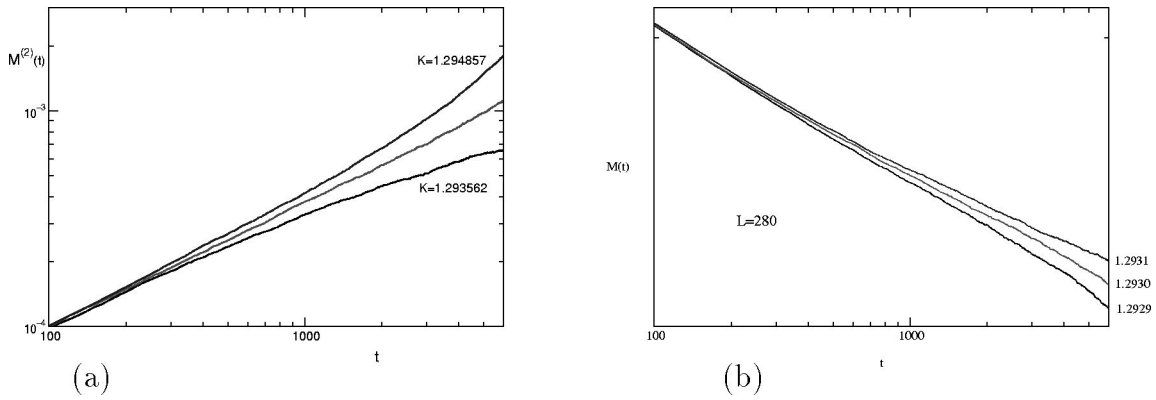

FIG. 1. Seven-state Potts model: (a) $M^{(2)}(t)$ on log-log scale for $K=1.293\,562$ (K_c), 1.294 210, and 1.294 857 (from below) with $L=280$. (b) $M(t)$ for $K=1.2929$, 1.2930, and 1.2931 (from below) with $L=280$.

servables present an approximate power law behavior. The *weaker* the transition is, the *cleaner* the power law behavior will be. This gives an estimate of K^*. Starting from a zero temperature state, for $K<K_c$ the system reaches the ordered metastable state first and one can determine K^{**}. In second-order transitions, K^* and K^{**} overlap with the transition point K_c. Therefore, a difference of K^* and K^{**} gives a criterion for a weak first-order transition.

For not too weak first-order transitions, the power law behavior of the observables will not be so clean and/or will not last a long time. Determination of K^* and K^{**} becomes somewhat ambiguous. But this is not a weak point of our method. If no power law behavior will be observed at any temperatures, it already indicates that the transition is not second order.

We first determine K^* for the seven-state Potts model. We consider a dynamic process in which the system initially in a *random* state is suddenly quenched to K_c or above, then evolves dynamically. We have performed simulations with the heat-bath algorithm. Lattice sizes are $L=140$ and 280 and maximum updating times are $t_{max}=2000$ and 6000, respectively. Total samples for averaging are 4600 and errors are simply estimated by dividing the data into four subsamples.

In Fig. 1(a), the second moment $M^{(2)}(t)$ with $L=280$ is displayed for $K=1.293\,562$ (K_c), 1.294 210, and 1.294 857 on a log-log scale. Apparently, at K_c the curve bends *downward* and does not show a power law behavior. But at a slightly bigger K, i.e. K^*, one observes an approximate power law behavior. When K becomes bigger than K^*, the curve bends *upward*. Therefore, K^* indeed looks like a critical point [12].

In the short-time dynamic approach, practically we locate the pseudo-critical-point K^* by interpolating $M^{(2)}(t)$ among the three simulated K's and searching for the best power law behavior [11,12]. In short-time critical dynamics, it has been intensively discussed that universal behavior emerges only after a time scale t_{mic} that is large enough in a microscopic sense. If a Monte Carlo time step (a sweep over all spins on the lattice) is a microscopic time unit, t_{mic} is typically 10 to some hundred time steps [12]. In first-order transitions, physical behavior at a *macroscopic* level is presented also only after t_{mic}. In the upper part of Fig. 2, K^* obtained with data in a time interval $[t,t_{max}]$ is shown. The results are stable and K^* is clearly above K_c. The final value for K^* is estimated to be $K^*_{7s}=1.293\,854(29)$. This is consistent with the value $K^*=1.2945(9)$ given in Ref. [26]. However, the latter can hardly distinguish K^* from K_c within the error.

To determine K^{**}, we study a dynamic process with an *ordered* initial state. We have performed extra simulations for $L=560$, up to $t_{max}=6000$. Total samples for $L=140$, 280, and 560 are 7000, 1500, and 135, respectively. In Fig. 1(b) the magnetization with $L=280$ is plotted for $K=1.2929$, 1.2930, and 1.2931. The curve for $K_c=1.293\,562$ (not in the figure) is much above that for 1.2931 and very far from power law behavior. However, at the pseudo-critical-point K^{**} we will observe approximate power law behavior. Searching for a curve with the best power law behavior from the three curves in Fig. 1(b), we determine the pseudo-critical-point K^{**}. The results are presented in the lower part of Fig. 2. The values are clearly below K_c.

Another interesting observable is the Binder cumulant $U(t)\equiv M^{(2)}(t)/[M(t)]^2-1$. If a transition is second order, $U(t)$ obeys a power law at the transition point. Therefore it can also be used for the determination of K^{**}. Results are included in Fig. 2. Summarizing all these measurements leads to $K^{**}_{7s}=1.293\,008(7)$.

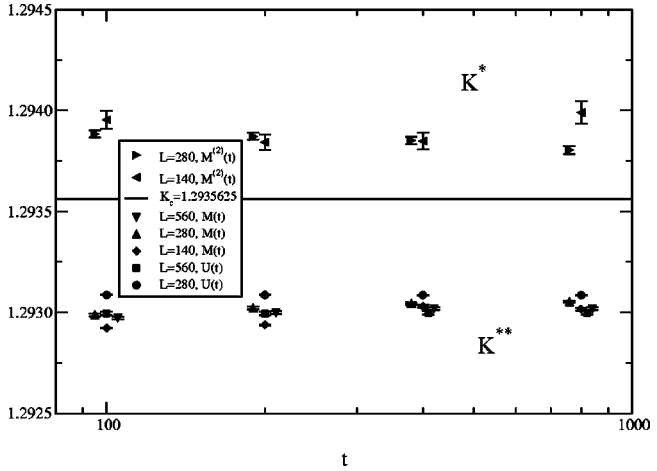

FIG. 2. Seven-state Potts model. The upper part shows K^* obtained from $M^{(2)}(t)$ in the interval $[t,t_{max}]$. The lower part shows K^{**} obtained from $M(t)$ and $U(t)$. The line denotes K_c.

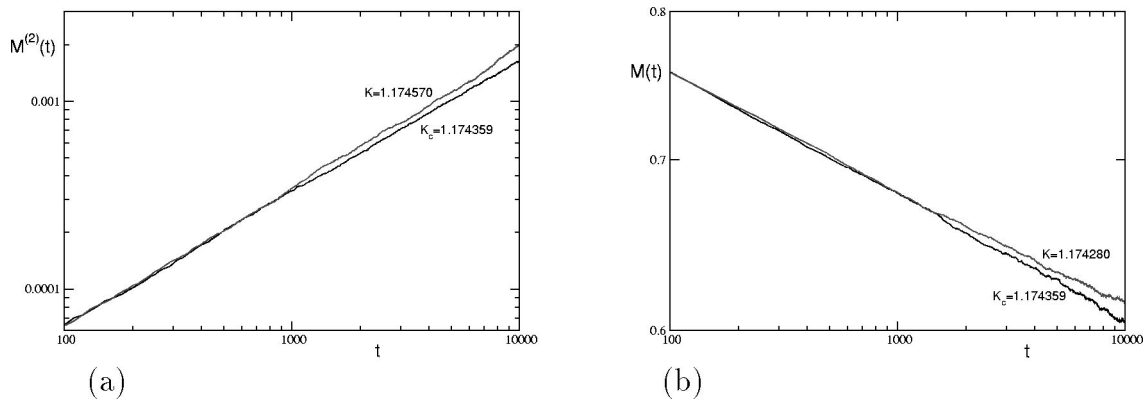

FIG. 3. Five-state Potts model: (a) $M^{(2)}(t)$ on log-log scale for $K_c=1.174\,359$ and $K=1.174\,570$ with $L=560$. (b) $M(t)$ for $K=1.174\,280$ and $K_c=1.174\,359$ with $L=560$.

For the five-state Potts model, the transition is extremely weak. One should carry out the simulations very carefully. To locate K^*, we have first performed simulations with $L=560$ for $K=1.174\,359$ (K_c), 1.174 946, and 1.175 533, up to $t_{max}=10\,000$ with 1800 samples. The resulting $K_{5s}^*=1.17\,445(6)$ is not accurate enough. Therefore another simulation has been carried out at $K=1.174\,570$, which is much closer to K^*. In Fig. 3(a), the second moments for $K=1.174\,359$ (K_c) and 1.174 570 are displayed. With these data, more accurate values for K^* are obtained and collected in the upper part of Fig. 4. We estimate the averaged $K_{5s}^*=1.174\,404(7)$.

Similar is the case for the determination of K^{**}. We have first performed simulations with an ordered initial state with $L=280$ and 560 for $K=1.173\,890$, 1.174 125, and 1.174 359 (K_c), up to $t_{max}=10\,000$ with total samples 725. From the data for the magnetization we estimate a rough $K_{5s}^{**}=1.17\,428(9)$. Then we performed simulations at $K=1.174\,280$ and 1.174 359 (K_c) up to $t_{max}=40\,000$. The results are not sensitive to whether we take $t_{max}=10\,000$ or 40 000. In Fig. 3(b), the magnetization at $K=1.174\,280$ and 1.174 359 (K_c) are plotted. From the lower part of Fig. 4, we obtain a final value $K_{5s}^{**}=1.174\,322(2)$.

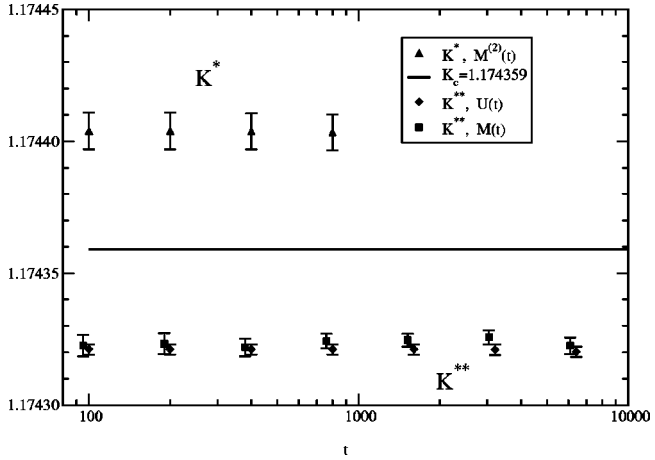

FIG. 4. Five-state Potts model. The upper part shows K^* obtained from $M^{(2)}(t)$ with $L=560$ in the interval $[t,t_{max}=10\,000]$. The lower part shows K^{**} obtained from $M(t)$ with $L=560$ in the interval $[t,t_{max}=40\,000]$. The line denotes K_c.

In Table I, all results for K^* and K^{**} have been collected. For both the seven-state and the five-state Potts model, K^* and K^{**} are clearly above and below the transition point K_c, respectively. Our short-time dynamic approach indeed provides a safe criterion for a weak first-order transition. For standard second-order transitions, K^* and K^{**} (i.e., K_c) determined from both dynamic processes overlap within errors [12]. Due to strong corrections to scaling, the four-state Potts model is known to be complicated in simulations in equilibrium. In short-time dynamics, our data also show that the measured K^* and K^{**} are relatively sensitive to the time interval for the measurements. But there are by no means signals that K^* is bigger than K^{**}.

Since our dynamic measurements are carried out in the short-time regime when the spatial correlation length is still short, we can easily control the finite-size effect. We also do not have the problem of generating independent configurations and therefore do not suffer from slowing down. After excluding the finite-size effect, the measurements are sensitive enough to distinguish a finite but very large spatial correlation length in equilibrium from an infinite one. This is why our method is successful.

With the pseudo critical points in hand, assuming similar scaling laws as in second-order transitions [12], one can estimate corresponding pseudo critical exponents. At K^*, e.g,

$$M^{(2)}(t)\propto t^{c_2},\quad c_2=(d-2\beta/\nu)/z. \tag{1}$$

At K^{**}, for the magnetization,

$$M(t)\propto t^{-c_1},\quad c_1=\beta/\nu z, \tag{2}$$

while for the Binder cumulant

$$U(t)\propto t^{c_U},\quad c_U=d/z. \tag{3}$$

TABLE I. Pseudo-critical-points K^{**} and K^* for the five-state and seven-state Potts models, in comparison with the transition point K_c.

	K^{**}	K_c	K^*
$q=5$	1.174322(2)	1.174359	1.174404(7)
$q=7$	1.293008(7)	1.293562	1.293854(29)

TABLE II. Pseudo critical exponents for the five-state and seven-state Potts models.

	c_1^{**}	c_U^{**}	c_2^{*}
$q=5$	0.091(2)	0.93(3)	0.716(3)
$q=7$	0.0239(2)	0.885(8)	0.502(5)

Here d is the dimension of the lattice, β and ν are static exponents, and z is the dynamic exponent. However, the values of the exponents at K^* and K^{**} can be different. Plotting the observables vs t in log-log scale, one measures the exponents from the slopes. The results are given in Table II. We admit that complete sets of exponents cannot be obtained so easily. One needs more careful simulations.

In conclusion, we have proposed a short-time dynamic approach to weak first-order transitions. From nonequilibrium short-time behavior of two dynamic processes starting from random and ordered initial states, pseudo critical points K^* and K^{**} are determined. Difference of K^* and K^{**} distinguishes a weak first-order transition from a second-order one. Since the measurements are carried out in short-time regimes, the method does not suffer from slowing down. Different from many techniques developed in simulations in equilibrium, our method is not based on the finite-size scaling.

A simple average of K^* and K^{**} gives a rather good estimate of the transition point K_c, especially for very weak transitions. For example, for the five-state Potts model $(K^*+K^{**})/2=1.174\,363$ and the relative deviation from the exact K_c is only the order of $O(10^{-6})$. It is interesting to investigate how to obtain an accurate K_c for not too weak transitions. Furthermore, how other relevant observables such as the specific heat and energy distribution evolve in nonequilibrium dynamics is also an important topic. It is challenging whether from short-time dynamics one can estimate the latent heat and the discontinuity of the order parameter in equilibrium.

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[1] H. K. Janssen, B. Schaub, and B. Schmittmann, Z. Phys. B: Condens. Matter **73**, 539 (1989).
[2] D. A. Huse, Phys. Rev. B **40**, 304 (1989).
[3] K. Oerding and H. K. Janssen, J. Phys. A **26**, 3369 (1993); **26**, 5295 (1993).
[4] K. Humayun and A. J. Bray, J. Phys. A **24**, 1915 (1991).
[5] D. Stauffer, Physica A **186**, 197 (1992).
[6] Z. B. Li, U. Ritschel, and B. Zheng, J. Phys. A **27**, L837 (1994).
[7] P. Grassberger, Physica A **214**, 547 (1995).
[8] L. Schülke and B. Zheng, Phys. Lett. A **204**, 295 (1995).
[9] B. Zheng, M. Schulz, and S. Trimper, Phys. Rev. Lett. **82**, 1891 (1999).
[10] Z. B. Li, L. Schülke, and B. Zheng, Phys. Rev. Lett. **74**, 3396 (1995).
[11] H. J. Luo, L. Schülke, and B. Zheng, Phys. Rev. Lett. **81**, 180 (1998).
[12] B. Zheng, Int. J. Mod. Phys. B **12**, 1419 (1998).
[13] K. Binder and D. W. Heermann, *Monte Carlo Simulation in Statistical Physics* (Springer, Berlin, 1992).
[14] C. Borgs and W. Janke, Phys. Rev. Lett. **68**, 1738 (1992).
[15] V. Privman, *Finite Size Scaling and Numerical Simulations of Statistical Systems* (World Scientific, Singapore, 1990).
[16] K. Binder, Rep. Prog. Phys. **60**, 487 (1997), and references therein.
[17] A. M. Ferrenberg and R. H. Swendsen, Phys. Rev. Lett. **61**, 2635 (1988).
[18] A. M. Ferrenberg and R. H. Swendsen, Phys. Rev. Lett. **63**, 1195 (1989).
[19] P. M. C. de Oliveira, S. M. M. de Oliveira, C. E. Cordeiro, and D. Stauffer, J. Stat. Phys. **80**, 1433 (1995).
[20] W. Janke and R. Villanova, Phys. Lett. A **209**, 179 (1995).
[21] A. M. Ferrenberg, D. P. Landau, and K. Binder, Phys. Rev. E **58**, 3353 (1998).
[22] J. Lee and J. M. Kosterlitz, Phys. Rev. Lett. **65**, 137 (1990).
[23] J. Lee, J. M. Kosterlitz, and E. Granato, Phys. Rev. B **43**, 11 531 (1991).
[24] W. Janke (private communication).
[25] P. de Gennes, *The Physics of Liquid Crystals* (Clarendon, Oxford, 1975).
[26] L. A. Fernández, J. J. Ruiz-Lorenzo, M. P. Lombardo, and A. Tarancón, Phys. Lett. B **277**, 485 (1992), and references therein.