Nonequilibrium critical relaxation of the order parameter and energy in the two-dimensional ferromagnetic Potts model

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The static and dynamic critical properties of the ferromagnetic q-state Potts models on a square lattice with $q=2$ and 3 are numerically studied via the nonequilibrium relaxation method. The relaxation behavior of both the order parameter and energy as well as that of the second moments are investigated, from which static and dynamic critical exponents can be obtained. We find that the static exponents thus obtained from the relaxation of the order parameter and energy together with the second moments of the order parameter exhibit a close agreement with the exact exponents, especially for the case of the $q=2$ (Ising) model, when care is taken in the choice of the initial states for the relaxation of the second moments. As for the case of $q=3$, the estimates for the static exponents become less accurate, but still exhibit reasonable agreement with the exactly known static exponents. The dynamic critical exponent for the $q=2$ (Ising) model is estimated from the relaxation of the second moments of the order parameter with *mixed* initial conditions to give $z(q=2)\simeq 2.1668(19)$.

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I. INTRODUCTION

The so-called nonequilibrium relaxation (NER) method [1,2] deals with the nonequilibrium critical relaxation of a statistical model instantaneously brought to its critical temperature from its nonequilibrium initial state, typically a fully ordered state. A unique feature about the NER method is that it allows one to determine the equilibrium critical properties of statistical systems from their *nonequilibrium* relaxation kinetics. Therefore, together with the method [3,4] using short-time critical dynamic properties [5,6] (see Sec. III D), the NER method has been an interesting and valuable tool to study the statistical systems whose critical properties are unknown.

With recent advances in computing power, it seems worthwhile to reinvestigate in more depth the potentials or limitations of the NER method in terms of numerical accuracies in static and dynamic exponents. In this work we chose the ferromagnetic q-state Potts model [7] on a square lattice (with $q=2$ and 3) as a testbed for the NER method. It appears to us that in applying the NER method, the energy relaxation itself has been overlooked in evaluating the critical exponents: previous works [8,9] employed mainly the second moments involving the energy, ignoring the relaxation of the energy itself. In this work we utilized the critical energy relaxation as well as that of the order parameter for evaluating the critical exponents. Due to better self-averaging of these single-moment quantities, higher accuracy is expected for the estimates of the exponents. Since for the ferromagnetic q-state Potts model the critical temperature and energy are exactly known for general values of q and the static critical exponents are exactly known for $q\leq 4$ [7,10], our work can be considered as a calibrational study of the NER method as to how accurate estimates for the critical exponents can be given via the NER method.

We find that by combining the relaxation of the two first-moment quantities—i.e., order parameter and energy—one can obtain the ratio of the equilibrium critical exponents, through which the nature of the phase transition, or, equivalently, the universality class, may be determined regardless of our knowledge of the exact value of the dynamic exponent z. By incorporating the time dependence of the second moment of the order parameter (starting from either disordered or ordered initial states), the dynamic exponent can be independently obtained. This can be combined with the relaxation of the first-moment quantities to give the two independent static exponents. We here find that the second moment of the order parameter obtained with disordered initial state gives the static exponents with higher accuracy. An alternative way of obtaining static exponents is to employ the second moments involving energy fluctuations. However, the energy fluctuation appears to be influenced by strong logarithmic corrections in the case of $q=2$, which makes it difficult to estimate the exponents with high accuracy.

The present work is motivated by our interest in applying the NER method to the statistical systems whose critical properties are not completely understood. We are particularly interested in clarifying the long-standing controversy on the critical properties of the fully frustrated XY (FFXY) model [11] on a square lattice [12] and the antiferromagnetic XY model [13] (or the antiferromagnetic clock model [14,15]) on a triangular lattice. Even though there exist previous studies [9,16–18] from a nonequilibrium dynamics perspective on this problem, we hope to undertake more careful studies of the FFXY model by applying the NER method with the strategy presented in this work.

II. MODEL AND SIMULATION METHOD

In the ferromagnetic q-state Potts model on a square lattice each spin σ_i can take one of q possible values $\sigma_i=1,2,\ldots,q$, and the spin interaction is defined by the Hamiltonian

TABLE I. The measured dynamic and static critical exponents.

		z	$1/\nu$	β	$\eta=2\beta/\nu$ $(d=2)$	$\alpha=2-\nu d$
$q=2$	Present work	2.1668(19)(z_{MM})	0.9984(25)	0.12527(51)	0.2501(16)	−0.0032(50)
	Short-time dynamics	2.155(3)	1.03(2)	0.1165	0.240(15)	0.058(38)
	Exact		1	1/8=0.125	1/4=0.25	0
$q=3$	Present work	2.1735(40) ($z_{MM,disordered}$)	1.213(6)	0.1080(20)	0.2618(83)	0.350(22)
	Short-time dynamics	2.196(8)	1.24(3)	0.1085	0.269(7)	0.387(40)
	Exact		6/5=1.2	1/9=0.1111	4/15=0.2666	1/3=0.3333

$$H = -J\sum_{\langle ij\rangle} \delta(\sigma_i,\sigma_j), \quad \sigma_i = 1,2,\ldots,q, \tag{1}$$

where $\delta(a,b)$ is the Kronecker delta function and $\langle ij\rangle$ denotes the nearest-neighbor spin pair. $J(>0)$ is the interaction strength.

The model is known to exhibit a continuous phase transition for $q\leq 4$ and discontinuous ones for $q>4$ in two dimensions [7]. For $q=2$, the Potts model is equivalent to the Ising model since $\delta(\sigma_i,\sigma_j)=(1+S_iS_j)/2$ with $S_i=\pm 1$. It is remarkable that though the model is not exactly solvable except for $q=2$, the critical temperature T_c and energy E_c are exactly known for general q in some two dimensional lattices. For the square lattice they are given by [7]

$$k_BT_c = \frac{J}{\ln(1+\sqrt{q})}, \quad E_c = -J\left(1+\frac{1}{\sqrt{q}}\right), \tag{2}$$

where k_B is the Boltzmann constant. Here and after we set $k_B=1$ and $J=1$. Hence $T_c=1.134\,59\ldots$ and $E_c=-1.707\,11\ldots$ for $q=2$ and $T_c=0.994\,97\ldots$ and $Ec=-1.577\,35$ for $q=3$. The exact static critical exponents are given in Table I.

We will be interested in characterizing the time evolution of the system instantaneously "heated" to T_c from a fully ordered initial state. The system then proceeds toward the equilibrium via Monte Carlo kinetics with the Metropolis algorithm for the flip of a randomly selected spin. Since we are interested in the long-time dynamics of the system in the thermodynamic limit, we take the system size large enough so that the simulation can appropriately mimic the nonequilibrium relaxation of the infinitely large system within the simulation time window. This is similar to the case of phase-ordering kinetics [19] in which the equilibration time is practically infinite due to large system size, making the time evolution ever in nonequilibrium. We use the square lattice with linear size $L=600$. The maximum simulation time is $t_{\max}=10^4$ Monte Carlo steps (MCS). The presented results are averages over 20 000 samples. Compared to existing dynamic studies [4,20–25] on the present model, our work has employed a larger lattice size with one or two decades longer Monte Carlo steps of simulations. Within the simulation time window, we have checked that there is no finite-size effect on our simulation results.

III. MEASUREMENTS AND DISCUSSIONS

We first define the local order parameter $m_i(t)$ and local energy $e_i(t)$ for the model and their respective sums $\mathcal{M}(t)$ and $\mathcal{E}(t)$ as

$$m_i(t) \equiv \frac{1}{(q-1)}[q\delta(\sigma_i(t),\sigma_i(0))-1],$$

$$e_i(t) \equiv -\frac{1}{2}\sum_j^{(i)} \delta(\sigma_i(t),\sigma_j(t)),$$

$$\mathcal{M}(t) \equiv \sum_i m_i(t), \quad \mathcal{E}(t) \equiv \sum_i e_i(t), \tag{3}$$

where $\Sigma_j^{(i)}$ denotes the sum over the nearest sites of site i. We have set $\sigma_i(0)=1$ in most of the present simulations. In the NER method, the determination of the critical exponents involves the cumulants of $\mathcal{M}(t)$ and $\mathcal{E}(t)$. The order parameter $M(t)$ and the energy density $E(t)$ are given by $M(t)\equiv\langle\mathcal{M}(t)\rangle/N$ and $E(t)\equiv\langle\mathcal{E}(t)\rangle/N$, respectively, where N is the total number of spins and the angular brackets $\langle\cdots\rangle$ denote an average over different realizations of the time evolution.

A. Locating the critical temperature and energy

The NER method provides us with an efficient tool to determine T_c with high accuracy. If the temperature T is above or below T_c, then the order parameter would relax (*stretched*) *exponentially* in time to its equilibrium value which is zero for $T\geq T_c$ or nonzero for $T<T_c$ in the continuous transition as in the present model. The relaxation time scale τ depends on how close T is to the critical temperature T_c. Approaching T_c, τ exhibits a power-law divergence. Below T_c, the order parameter $M(t)$ relaxes toward the nonvanishing equilibrium value. Since only at T_c does the order parameter exhibit a power-law relaxation, T_c can be located as the temperature at which the order-parameter relaxation gives the best straight line in a log-log plot of $M(t)$ versus t. A more accurate location of T_c naturally requires a longer simulation time.

Since T_c is exactly known for the present model, we can provide a test example as to how the order-parameter relaxation can be used to narrow down the critical temperature, as shown in Fig. 1(a) $(q=2)$ and Fig. 1(b) $(q=3)$. Figure 1(a) shows the relaxation of the Ising $(q=2)$ order parameter for

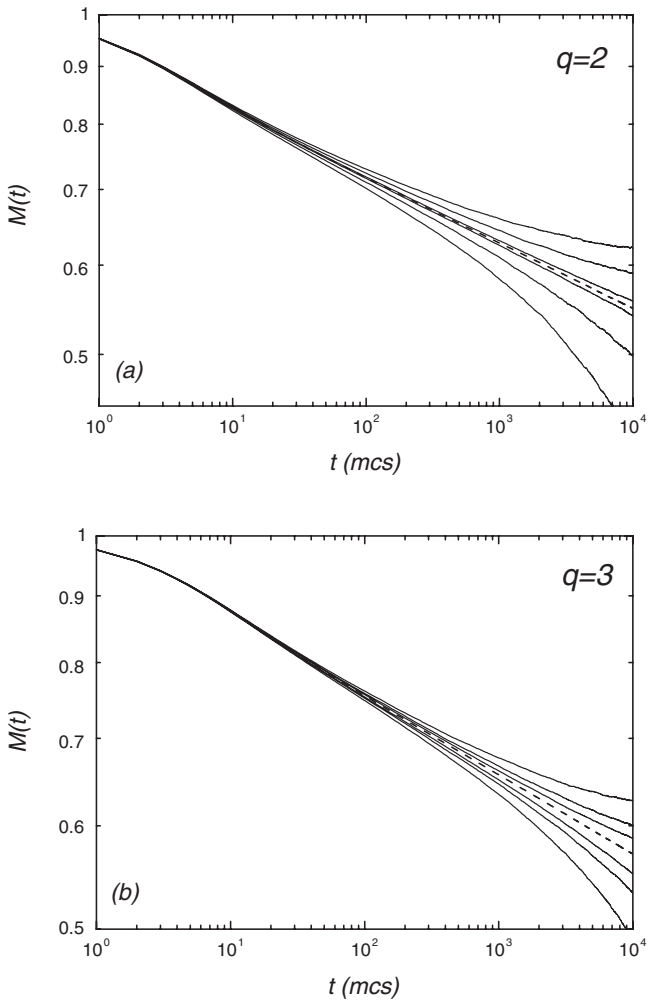

FIG. 1. The relaxations of the order parameter $M(t)$ for (a) $q=2$ and for (b) $q=3$ at temperatures near T_c [(a) $T=1.130$, 1.1323, 1.1342, 1.13459(T_c), 1.135, 1.137, and 1.14 and (b) $T=0.993$, 0.994, 0.9945, 0.99497(T_c), 0.9955, 0.996, and 0.997]. The critical temperature can be determined as the temperature at which $M(t)$ exhibits a critical relaxation (represented by a dashed line) through a change from an upward curvature to a downward curvature.

various temperatures near T_c. $M(t)$ shows strong upward and downward curvatures at $T=1.13$ and at $T=1.14$, respectively. So the critical temperature should be in the range $1.13<T_c<1.14$. We find in this way that the temperature range can be readily narrowed down to $\delta T=4\times10^{-4}$ within the present simulation time ($t_{\max}=10^4$ MCS). That is, we have $1.1342<T_c<1.1350$. Higher accuracy would be achieved with a longer simulation time. In the same manner, for $q=3$, T_c can be easily located within the range $\delta T=5\times10^{-4}$ as demonstrated in Fig. 1(b).

In contrast to the case of the present system, the exact value of the critical energy is not known for many other systems. For such cases, using an ansatz of the critical energy relaxation at T_c, one can determine E_c by tuning the value of E^* such that $E^*-E(t)$ versus t gives the best straight line at long times in the log-log plot. Figure 2 shows such an example for the present system. In our simulation time window, one could readily narrow down E_c within the range $\delta E\simeq10^{-3}$.

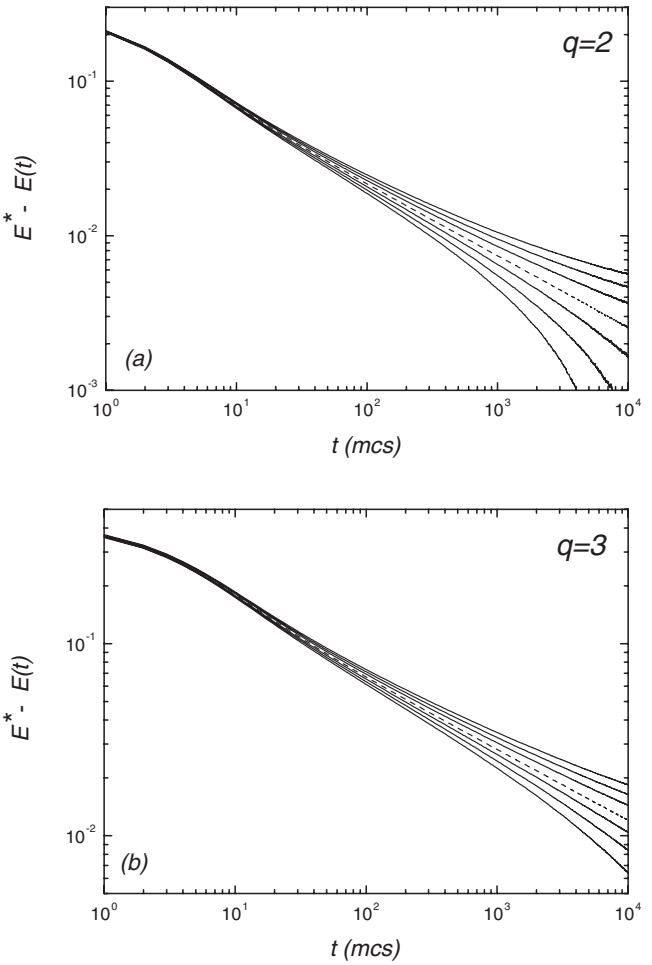

FIG. 2. The relaxations of the energy difference $[E^*-E(t)]$ in a log-log plot for (a) $q=2$ and (b) $q=3$ with various test values of E^* [(a) $E^*=-1.704$, -1.705, -1.706, $-1.70711(E_c)$, -1.708, -1.709, and -1.710 and (b) $E^*=-1.571$, -1.573, -1.575, $-1.57735(E_c)$, -1.579, -1.581, and -1.583]. By tuning E^* such that $E^*-E(t)$ exhibits the best power-law relaxation, one can determine both E_c and $-(\nu d-1)/z\nu$. For each figure, the dashed line represents the relaxation with the exact critical energy E_c.

B. Relaxations of the first moments

We first measure the relaxation of the order parameter $M(t)$ and the energy density $E(t)$. When the system is instantaneously brought to T_c starting from a fully ordered state, both quantities exhibit power-law relaxations toward their equilibrium values [8,26,27]. For a better analysis of the relaxation behavior and estimation of the critical exponents, we included correction terms to the leading-order scaling behavior in the following form (see the Appendix for a derivation of the leading-order critical relaxation):

$$M(t)\sim t^{-\beta/z\nu}\left(1+\frac{c_M}{t^{\delta_M}}+\frac{c'_M}{t^{\delta'_M}}+\frac{c''_M}{t^{\delta''_M}}+\cdots\right),$$

$$E_c-E(t)\sim t^{-(\nu d-1)/z\nu}\left(1+\frac{c_E}{t^{\delta_E}}+\frac{c'_E}{t^{\delta'_E}}+\frac{c''_E}{t^{\delta''_E}}+\cdots\right), \quad (4)$$

where z is the dynamic exponent, β and ν the static exponents, and d the spatial dimension ($d=2$ in the present case).

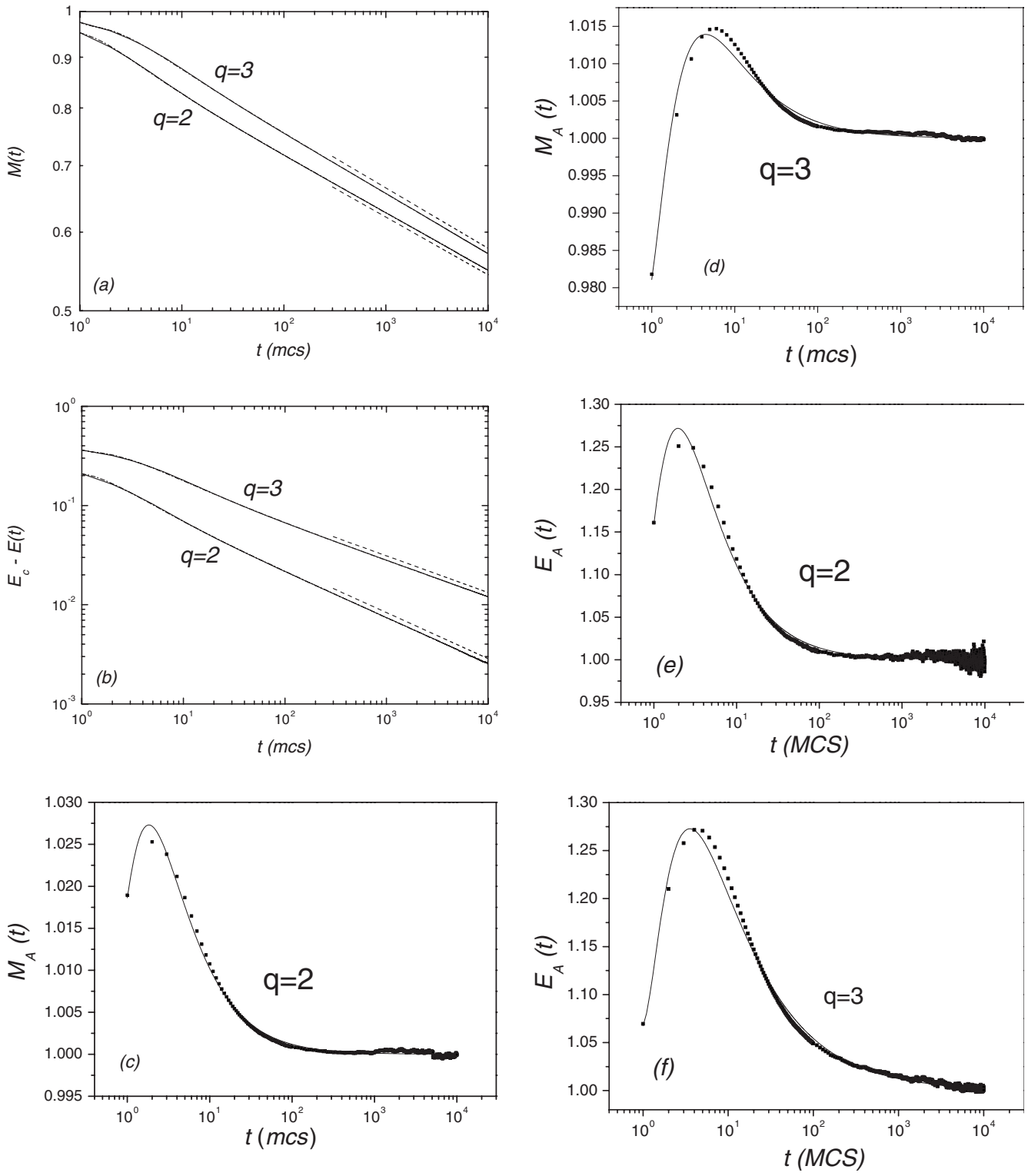

FIG. 3. (a) The critical relaxation of the order parameter $M(t)$ and (b) the critical relaxation of the energy difference $[E_c - E(t)]$. In (a) and (b) dot-dashed lines are curves obtained from FIT3A with optimal fits. Shown in (c) and (d) are plots of $M_A(t) \equiv M(t)A_0 t^{\beta/z\nu}$ (solid square) together with the fitting function (solid line) for $q=2$ and $q=3$, respectively. Here $A_0^{-1} t^{-\beta/z\nu}$ represents the asymptotic scaling obtained from the fitting. Shown in (e) and (f) are the plots of $E_A(t) \equiv [E_c - E(t)]B_0 t^{(\nu d-1)/z\nu}$ vs t (solid square) together with the fitting function (solid line) for $q=2$ and $q=3$, respectively. Here $B_0^{-1} t^{-(\nu/d-1)/z\nu}$ represents the asymptotic scaling obtained from the fitting.

In (4), c_M, c'_M, c''_M and c_E, c'_E, c''_E are constants, and δ_M, δ_E, etc., are the exponents of the correction-to-scaling terms. Simulation results for the relaxations of $M(t)$ and $E_c - E(t)$ are shown, respectively, in Figs. 3(a) and 3(b).

It is easy to see that the general form of Eq. (4) with all the correction exponents kept independent is not appropriate

for fitting. For example, if we put all the correction exponents equal to one another, then we can generate the same function with many different combinations of the coefficients provided that the sums of the coefficients are the same. This will cause the fitting procedure with a general initial guess to fail to converge to unique stable values for the values of exponents and other coefficients. Therefore, we should impose some constraints on the correction exponents to achieve a stable fit. One of the schemes we tried is to let the first correction exponent be a free fitting parameter, but the nth correction exponent is constrained to be equal to the first correction exponent plus $(n-1)$. That is, we put $\delta'_M=\delta_M+1$ and $\delta''_M=\delta_M+2$, etc. (which we call FITnA, where n refers to the number of correction terms). We also tried a scheme where the first correction exponent is a free-fitting parameter, but the nth correction exponents are constrained to be equal to n times the first correction exponent. That is, we put $\delta'_M=2\delta_M$ and $\delta''_M=3\delta_M$, etc. (which we call FITnC). A special scheme of correction is to assume an analytic form for the correction terms where the correction exponents are all constrained to integer values (which we call FITnB). The cases of $\delta_M=1$ in FITnA and FITnC reduce to the scheme of FITnB. The special case of fitting with a simple power law without correction terms will be referred to as FIT0.

First consider the case of $q=2$. In this case, we incorporated up to third correction terms (i.e., FIT3A, FIT3C, and FIT3B) in our fit. In the cases of FIT3A and FIT3C, for reasonable convergence of the fitting procedure and estimation of the error bars, we tuned the value of the coefficients of the highest-order correction terms (i.e., c''_M and c''_E). These values of c''_M and c''_E were tuned (chosen) such that the resulting fit function shows good agreement with the data. For some finite range of these coefficient values (c''_M ranging from 0.0 to 0.1), the quality of the fit is found to be acceptable. The median of the values of the exponents was chosen as the representative value of the exponent, and the range of the values can be used to estimate the error bars. As for the relaxation of the magnetization, we found that, as the value of c''_M was varied, the value of the dominant relaxation exponent $\beta/z\nu$ showed only a small variation. We also found that, in terms of the value of the dominant exponent $\beta/z\nu$ and the first correction exponents, the two schemes of FIT3A and FIT3C gave almost the same results (see Table II). If we take the median of the fitted values from this analysis as the most probable value of $\beta/z\nu$, we get

$$\frac{\beta}{z\nu}=0.057722(42) \quad \text{for } q=2. \tag{5}$$

Now the corresponding value of the first correction exponent δ_M from the above fit exhibits a monotonic increase from 0.91 to 1.06 (FIT3C) and also from 0.90 to 1.07 (FIT3A) as the value of c''_M increases from 0.0 to 0.1 (Table II). Taking the median of the combined range (from 0.90 to 1.07) we may take the representative value of δ_M as $\delta_M\simeq 0.985(85)$. This may indicate that the exact value of the first correction exponent is equal to 1. Incidentally we also tried to fit the data with analytic corrections in which the first correction exponent is set to be equal to 1, the second correction exponent to 2, etc. We found that the fitting quality was excellent with essentially the same dominant exponent as the representative value given above.

TABLE II. The dominant exponents and the first correction exponents for the relaxation of magnetization, obtained from the two fitting procedures FIT3A and FIT3C for the case of $q=2$. z_M denotes the value of the dynamic exponent derived from the value of the second column for $\beta/z\nu$ using the exact values of the static exponents for β and ν. c''_M represents the chosen values of the coefficients of the highest-order correction terms for fits. For comparison, we also added (the last line) the result of a fit with FIT3B where the first correction exponent δ_M is set equal to unity.

	c''_M	$\beta/\nu z$	δ_M	z_M
FIT3A	0.0	0.0576815	0.8956	2.16707
	0.01	0.0576911	0.9165	2.16671
	0.02	0.0577003	0.9366	2.16637
	0.03	0.0577094	0.9559	2.16603
	0.04	0.0577181	0.9745	2.16570
	0.05	0.0577266	0.9924	2.16538
	0.07	0.0577427	1.0265	2.16478
	0.1	0.0577652	1.0738	2.16393
FIT3C	0.0	0.05768	0.907	2.1671
	0.01	0.057689	0.9264	2.16679
	0.02	0.057699	0.9442	2.16642
	0.03	0.057708	0.9612	2.16606
	0.04	0.057717	0.9774	2.16573
	0.06	0.0577338	1.0078	2.16511
	0.08	0.0577494	1.0363	2.16453
	0.1	0.0577642	1.0633	2.16397
FIT3B	0.07834	0.05769	1.0 (fixed)	2.16675

As for the relaxation of the excess energy, we also applied the above fitting schemes. However, in this case of excess energy, we had to directly tune the value of the first correction exponent in order to obtain a reasonable fit to the data. We found that the best fit could be obtained in the range of the value of δ_E between 0.90 and 1.05 (see Table III) which again is in reasonable agreement with the case of the magnetization relaxation [Fig. 3(b)]. The values of the fitted relaxation exponents are

$$\frac{\nu d-1}{z\nu}=0.46227(71) \quad \text{for } q=2. \tag{6}$$

Now we turn to the relaxation dynamics of the $q=3$ model. As for the magnetization relaxation, we tuned the value of the coefficient c''_M or c''_E of the highest-order correction terms. We find that both schemes FIT3A and FIT3C give approximately the same results for values of the relaxation exponent $\beta/z\nu$ (Table IV). Combining the results of FIT3A and FIT3C we obtain the values of the exponent as

$$\frac{\beta}{z\nu}=0.06020(17) \quad \text{for } q=3. \tag{7}$$

Correspondingly the value of the first correction exponent δ_M ranges between 0.65 and 0.98. As for the relaxation of the

TABLE III. The dominant exponents and the first correction exponents for the energy relaxation, obtained from the two fitting procedures FIT3A and FIT3C for the case of $q=2$. Note that z_E denotes the value of the dynamic exponent derived from the value of the second column for $(\nu d-1)/\nu z$ using the exact value of the static exponents for ν. Here the exponent δ_E's represent the chosen values of the first correction exponents for fitting.

	δ_E	$(\nu d-1)/\nu z$	c_E''	z_E
FIT3A	0.90	0.46201	0.2028	2.1645
	0.95	0.46227	0.47124	2.1632
	1.0	0.46253	0.76616	2.1620
FIT3C	0.93	0.462169	0.26146	2.1637
	0.95	0.462265	0.40190	2.1633
	0.96	0.462315	0.47326	2.1630
	0.97	0.462367	0.54537	2.1628
	1.0	0.462530	0.766162	2.1620

excess energy, we also applied the above fitting schemes. We found that the best fit could be obtained in the range of the value of δ_E between 0.6 and 0.74 which exhibits a narrower range for the correction exponent compared with the case of magnetization relaxation. The value of the fitted relaxation exponent for excess energy is (Table V)

$$\frac{\nu d-1}{z\nu}=0.3626(40) \quad \text{for } q=3. \tag{8}$$

Figures 3(c) and 3(d) show the time dependence of $M_A(t) \equiv M(t)A_0 t^{\beta/z\nu}$ for $q=2$ and $q=3$, respectively, together with the fitting functions. Here $A_0^{-1}t^{-\beta/z\nu}$ represents the asymptotic scaling obtained from the fitting. Also, Figs. 3(e) and 3(f) show the time dependence of $E_A(t) \equiv [E_c - E(t)]B_0 t^{(\nu d-1)/z\nu}$ with the fitted values of the exponents for $q=2$ and $q=3$, respectively, together with the fitting functions, demonstrating the asymptotic nature of the scaling behaviors. Here $B_0^{-1}t^{-(\nu/d-1)/z\nu}$ represents the asymptotic scaling obtained from the fitting.

TABLE IV. The dominant exponents and the first correction exponents for the relaxation of magnetization, obtained from the two fitting procedures FIT3A and FIT3C for the case of $q=3$. c_M'' represents the chosen values of the coefficients of the highest-order correction terms for fits. Also shown in the last two lines are the results of fits using FIT3B and FIT0 (with no correction terms), respectively.

	c_M''	$\beta/\nu z$	δ_M	z_M
FIT3A	0.03	0.0600345	0.6415	2.2209
	0.06	0.0601009	0.7063	2.2185
	0.07	0.0601192	0.7260	2.2178
	0.08	0.0601374	0.7451	2.2171
	0.09	0.060154	0.7634	2.2165
	0.10	0.060170	0.7811	2.2159
	0.12	0.0601995	0.8149	2.2149
	0.15	0.060241	0.8630	2.2133
FIT3C	0.06	0.060141	0.7713	2.2170
	0.09	0.060183	0.8139	2.2155
	0.10	0.0601959	0.8274	2.2150
	0.12	0.0602175	0.8524	2.2142
	0.15	0.060249	0.88845	2.2130
FIT3B	0.244	0.0603559	1.0 (fixed)	2.2091
FIT0	-	0.06058	-	2.2010

TABLE V. The dominant exponents and the first correction exponents for the energy relaxation, obtained from the two fitting procedures FIT3A and FIT3C for the case of $q=3$. Here the exponents δ_E represent the chosen values of the first correction exponents for fits.

	δ_E	$(\nu d-1)/\nu z$	c_E''	z_E
FIT3A	0.55	0.36008	0.3898	2.2218
	0.60	0.36142	0.6459	2.2135
	0.61	0.36167	0.6997	2.2119
	0.62	0.36192	0.7544	2.21045
	0.63	0.36216	0.8099	2.20899
	0.64	0.36239	0.8664	2.20756
FIT3C	0.70	0.36298	0.7896	2.20397
	0.72	0.36336	0.9676	2.20165
	0.73	0.36356	1.057	2.2005
	0.74	0.36375	1.1464	2.1993

Note that the value of $\beta/z\nu$ is particularly small. This implies that the order parameter relaxes much more slowly than the energy does: even after four decades of relaxation time, the order parameter relaxed only half of its initial value. This is another reason why the statistics is better for the order parameter relaxation than for the energy relaxation. The above values of $\beta/z\nu$ for both $q=2$ and 3 can be compared with the results obtained from the short-time dynamics on both square [4,21] and triangular [25] lattices.

Since $\beta/z\nu$ and $(\nu d-1)/z\nu$ contain the common factor $1/z\nu$ which involves the dynamic critical exponent z, taking the ratio of the former to the latter eliminates the exponent z, yielding $\beta/(\nu d-1)$ which involves only the two static exponents. Then the numerical values of the ratio $\beta/(\nu d-1)$ obtained from the above fit can be compared with the corresponding exact values as

$$\frac{\beta}{\nu d-1}=0.1249(4),$$

$$\left(\frac{\beta}{\nu d-1}\right)_{\text{exact}}=\frac{1}{8}=0.125 \quad \text{for } q=2,$$

$$\frac{\beta}{\nu d-1}=0.1660(23),$$

$$\left(\frac{\beta}{\nu d-1}\right)_{\text{exact}}=\frac{1}{6}=0.16667 \quad \text{for } q=3. \tag{9}$$

We see that for both cases of $q=2$ and $q=3$, the values of $\beta/(\nu d-1)$ are quite close to the exact theoretical values.

Elimination of the dynamic exponent z in the above ratio is an important feature that may be used to distinguish the universality class of systems whose critical properties are not known. Prominent examples of such systems are the two-dimensional FFXY models [12]. We point out that as is done here, measuring the relaxations of the chirality order parameter and the energy for such systems one can determine whether the chirality transition in that system belongs to the Ising or the three-state Potts universality class, or to another universality class, without knowing all the static exponents separately.

One can obtain an estimate for z from the fitted exponents for the relaxation of magnetization and energy as given above by making use of the fact that the static exponents are exactly known in the case of $q=2$ and $q=3$. This is perhaps one of the easiest ways of obtaining z for systems whose static critical properties are exactly known [28,29]. If we use the magnetization relaxation, the values for z derived from the values of the relaxation exponents in (5)–(8) (assuming the exact theoretical values of the static exponents) are given by

$$z_M = 2.1656(16), \quad z_E = 2.1632(33) \quad \text{for } q = 2,$$

$$z_M = 2.2150(62), \quad z_E = 2.2064(110) \quad \text{for } q = 3. \quad (10)$$

Here values of the exponents are the median values in the optimal fitting regime, while the error bars are estimated from the maximum dispersion of the fitted values. The values of z in (10) are in good accord with other estimates [30].

C. Relaxations of the second moments

The above procedures of obtaining z of course cannot be carried out for systems with unknown critical properties. It is thus desirable to provide ways of independently measuring the dynamic exponent. We present below one systematic way of doing it by considering the second moments of the order parameter, $C_{\mathcal{MM}}(t)$, which exhibits a leading-order scaling behavior in time [8] as (see the Appendix)

$$C_{\mathcal{MM}}(t) \equiv N[\langle \mathcal{M}^2(t)\rangle - \langle \mathcal{M}(t)\rangle^2] \sim t^{(d-2\beta/\nu)/z}. \quad (11)$$

Note that (11) is valid for *disordered* initial states as well. The dynamic exponent z can be isolated if one considers a time-dependent second moment $f_{\mathcal{MM}}(t)$ defined as

$$f_{\mathcal{MM}}(t) \equiv \frac{C_{\mathcal{MM}}(t)}{M^2(t)} \sim t^{d/z}, \quad (12)$$

which is obtained using the leading-order behavior for $M(t)$ given in (4). One usually measures $f_{\mathcal{MM}}(t)$ in two ways: one measures $f_{\mathcal{MM}}(t)$ for fully ordered initial states, or one can first measure $C_{\mathcal{MM}}(t)$ for disordered initial states and then divide it by $M^2(t)$ measured for the fully ordered initial states. The latter way is therefore using the two different types of initial conditions. We denote the former result by $f_{\mathcal{MM},ordered}(t)$ and the latter one by $f_{\mathcal{MM},mixed}(t)$. An alternative way [4] of obtaining z using the short-time critical dynamics is described in the next section.

Shown in Figs. 4(a) and 4(b) are $f_{\mathcal{MM}}(t)$ for $q=2$ and $q=3$, respectively. Here, we apply similar methods of analysis as in the previous section—that is, $f_{\mathcal{MM}}(t) \sim t^{d/z}(1 + c_{\mathcal{MM}}/t^{\delta_{\mathcal{MM}}} + \cdots)$. We found that for the case $q=2$ (using both FIT2A and FIT2C) $f_{\mathcal{MM},ordered}(t)$ and $f_{\mathcal{MM},mixed}(t)$ give (Tables VI and VII)

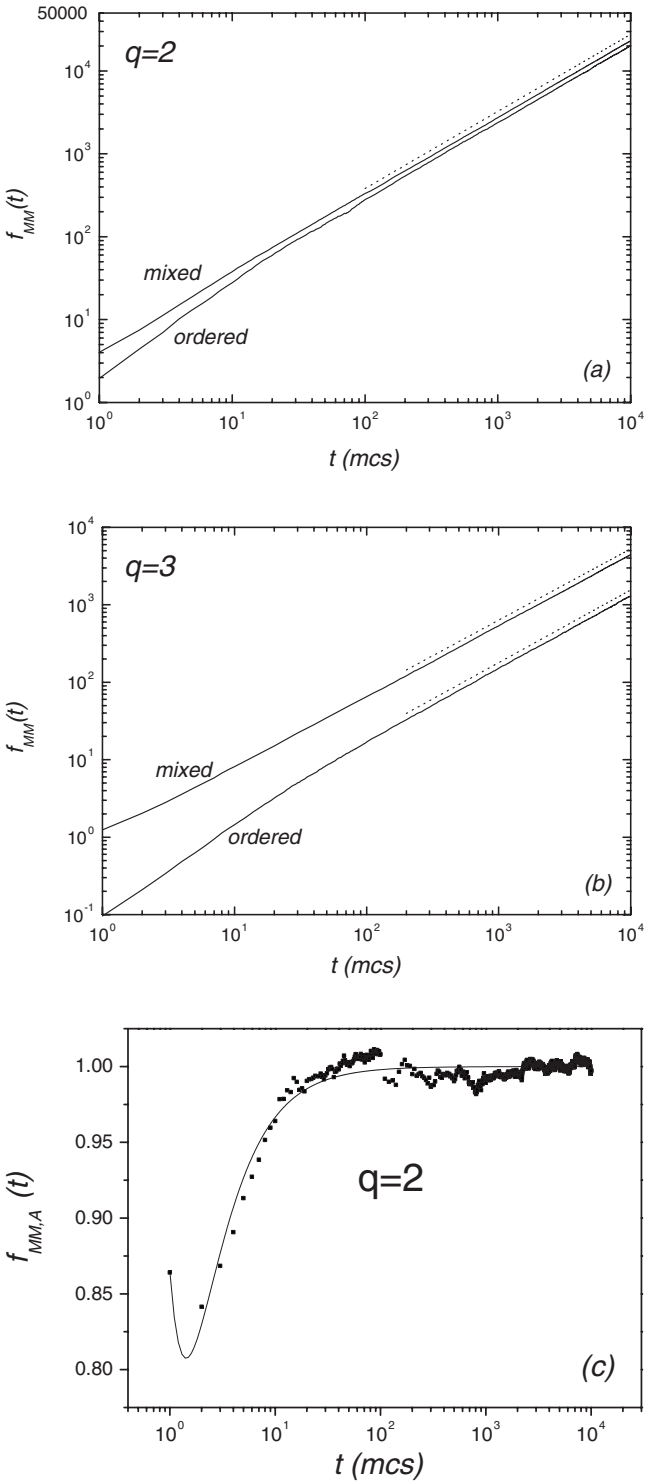

FIG. 4. The order-parameter cumulant $f_{\mathcal{MM}}(t)$ vs t in a log-log plot for $q=2$ (a) and $q=3$ (b). (c) $f_{\mathcal{MM},A}(t) \equiv f_{\mathcal{MM}}(t) C_0 t^{-d/z}$ vs t in the case of mixed initial states for $q=2$ (solid square) together with the fitting function (solid line). Here $C_0^{-1} t^{d/z}$ represents the asymptotic scaling obtained from the fitting. Dotted lines are the straight lines indicating the asymptotic power-law behavior.

TABLE VI. The dominant exponents and the first correction exponents for the relaxation of the second moment of magnetization with *random* initial states, obtained from the two fitting procedures FIT3A and FIT3C for the case of $q=2$. Here, the fitting is mostly done up to second corrections. c''_{MM} is the chosen values of the coefficients of the highest-order correction terms for fits.

	δ_{MM}	c''_{MM}	d/z	z_{MM}
FIT3A	1.35	0.0	0.92323	2.16631
	1.3	0.0	0.92311	2.16659
	1.25	0.0	0.92298	2.16689
	1.20	0.0	0.92285	2.16720
	1.15	0.0	0.92271	2.16753
	1.0	0.6923	0.92314	2.16652
	1.0	0.0	0.92224	2.16863
FIT3C	1.34595	0.0	0.92335	2.16603

$$z_{ordered} = 2.1545(52), \quad z_{mixed} = 2.1668(19) \quad \text{for } q = 2. \tag{13}$$

We see that there exists a small but non-negligible discrepancy between the exponents z_{mixed} and $z_{ordered}$. We also note in particular that z_{mixed} is very close to z_M obtained from the relaxation of the magnetization in (5) (assuming the exact values of the static exponents). Figure 4(c) shows the time dependence of the quantity $f_{\mathcal{MM},A}(t) \equiv f_{\mathcal{MM}}(t) C_0 t^{-d/z}$ for the case of mixed initial states (for $q=2$) together with the fitting function, where $C_0^{-1} t^{d/z}$ represents the asymptotic scaling obtained from one of the best fits.

In the case of $q=3$, $z_{ordered}$ and z_{mixed} exhibit a larger discrepancy:

$$z_{ordered} = 2.1334(35), \quad z_{mixed} = 2.1735(40) \quad \text{for } q = 3. \tag{14}$$

As first pointed out by Zheng [4], this difference between the two estimates is not due to the statistical error of the data. This difference is also observed in triangular lattices [25]. More severe disagreement between $z_{ordered}$ and z_{mixed} was reported for the Baxter-Wu model [32,33]: $z_{ordered}=2.07(1)$ [34] and $z_{mixed}=2.294(6)$ [35]. We suspect that the underlying reason for this discrepancy is that the time scale at which the scaling behavior sets in may be much longer for $f_{\mathcal{MM},ordered}(t)$ than that for $f_{\mathcal{MM},mixed}(t)$ as q gets larger, which may be due to the nature of the broken symmetry of the initial states related to the higher degeneracy of the ground states for larger q. It is thus expected that the stronger discrepancy will be observed for the four-state Potts model as well [36,37].

TABLE VII. The dominant exponents and the first correction exponents for the relaxation of the second moment of magnetization with *ordered* initial states, obtained from the two fitting procedures FIT2A and FIT0 for the case of $q=2$. The column for c'_{MM} lists the chosen values of the coefficients of the second correction terms for fits.

	δ_{MM}	c'_{MM}	d/z	z_{MM}
FIT2A	0.8317	0.15	0.927756	2.15574
	0.8471	0.09	0.927876	2.15546
	0.8545	0.06	0.927933	2.15533
	0.8618	0.03	0.927988	2.15520
	0.8689	0.0	0.928042	2.15507
	0.8713	−0.01	0.92806	2.15503
FIT0	-	-	0.92819	2.15473

Static exponents ν and β

The values of dynamic critical exponents obtained from second moments of the order parameter can now be combined with the relations of exponents obtained from the relaxation of the first moments of the order parameter and energy to give the static exponents such as ν and β. Since it appears that the value of z_{mixed} (especially for $q=2$) is more consistent with the results of magnetization and energy relaxation, we substituted z_{mixed} for the dynamic exponents in the relaxation of magnetization and energy. For example, in the case of $q=2$, substituting the value of $z_{mixed}=2.1668(19)$ in (13) for z in the relations (5) and (6) gives $1/\nu=0.9984(25)$ and $\beta=0.12527(51)$. These values yield close estimates to the exact exponents: $1/\nu=1$ and $\beta=1/8=0.125$.

As for $q=3$, when the value of $z_{mixed}=2.1735(40)$ in (14) is substituted for z in the relations (7) and (8) we obtain $1/\nu=1.212(16)$ and $\beta=0.1080(20)$, which appears to exhibit approximate agreement with the exact values $1/\nu=6/5=1.2$ and $\beta=1/9=0.1111$. But this is definitely less accurate than the case of $q=2$. If we use $z_{ordered}$ instead of z_{mixed}, then we obtain even less accurate results for the static exponents, which is naturally expected from the discrepancy of the value of $z_{ordered}$ from z obtained from the relaxation of the order parameter or energy assuming the exact static exponents. One thus should be cautious in determining z from second and higher moments of the order parameter for systems with unknown critical properties.

We have so far followed the procedure of using the relaxations of the order parameter, the energy, and the second moment of the order parameter. An alternative way [8,9] of obtaining the exponent ν is to use the second-order moments involving energy fluctuations, $f_{\mathcal{ME}}(t)$ or $f_{\mathcal{EE}}(t)$, which exhibit the leading-order scaling behaviors as [8] (see the Appendix)

$$f_{\mathcal{ME}}(t) \equiv N\left[\frac{\langle \mathcal{M}(t)\mathcal{E}(t)\rangle - \langle \mathcal{M}(t)\rangle\langle \mathcal{E}(t)\rangle}{\langle \mathcal{M}(t)\rangle\langle \mathcal{E}(t)\rangle}\right] \sim t^{1/z\nu},$$

$$f_{\mathcal{EE}}(t) \equiv N\left[\frac{\langle \mathcal{E}^2(t)\rangle - \langle \mathcal{E}(t)\rangle^2}{\langle \mathcal{E}(t)\rangle^2}\right] \sim t^{\alpha/z\nu}. \tag{15}$$

For $q=2$, we first obtain the leading-order exponent $1/z\nu=0.4624(29)$ by using FIT3A [Fig. 5(a)]. However, we are unable to extract the exponent $(2-\nu d)/z\nu$ from $f_{\mathcal{EE}}(t)$ since it exhibits a strong curvature with the local slope decreasing in time, as shown in Fig. 5(b). This may indicate that the exponent $(2-d\nu)$ eventually vanishes in the long-time limit, implying $\nu=1$. We suspect that this strong curvature in the log-

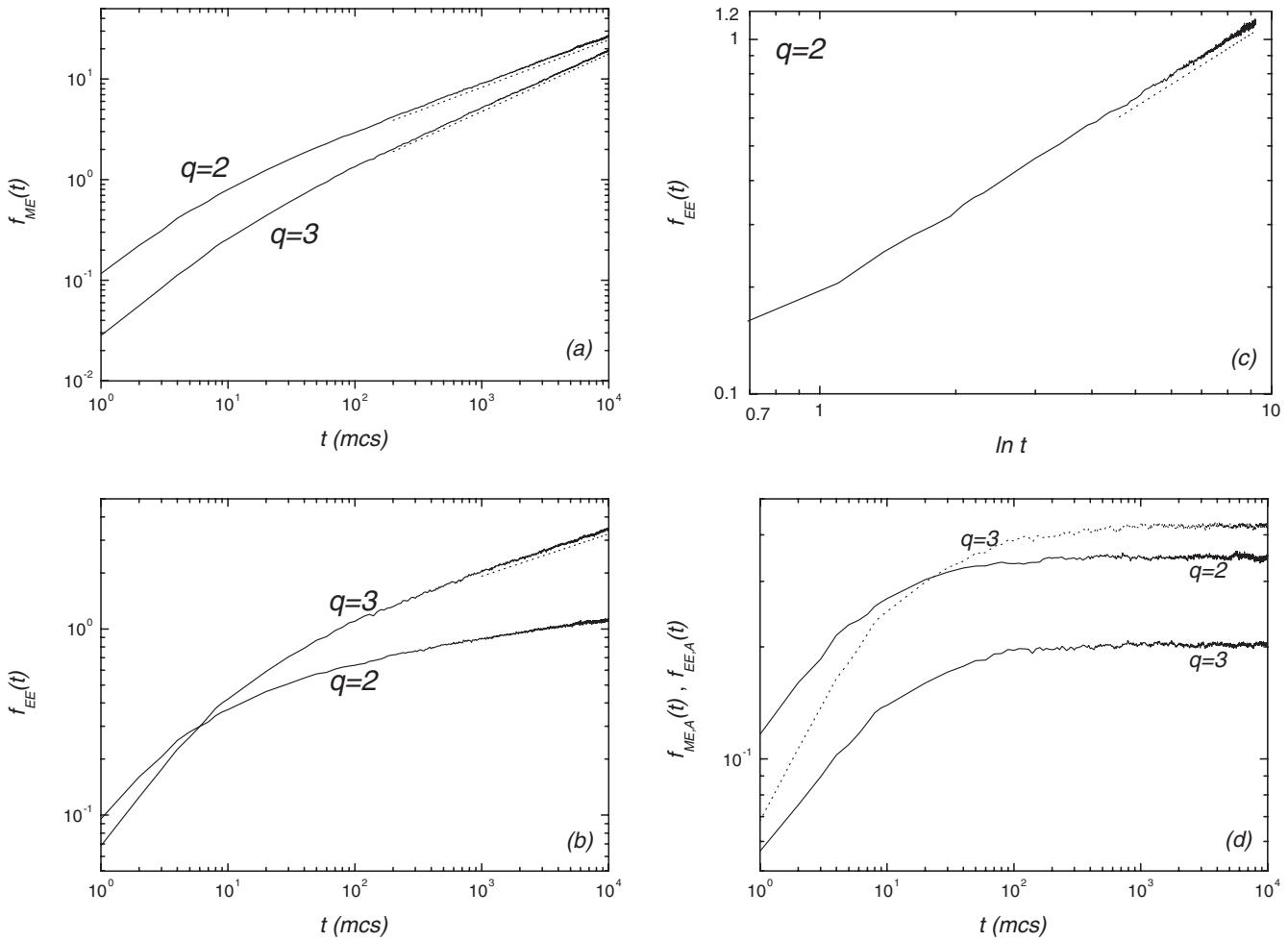

FIG. 5. The second-order moments $f_{\mathcal{ME}}(t)$ (a) and $f_{\mathcal{EE}}(t)$ (b) vs t in a log-log plot for $q=2$ and $q=3$. (c) $f_{\mathcal{EE}}(t)$ vs $\ln t$ in a log-log plot for $q=2$. This plot shows a logarithmic time dependence of $f_{\mathcal{EE}}(t) \sim (\ln t)^{\phi}$ with $\phi \simeq 0.80$ for the long-time region [$t \geq 100$ (MCS)].

log plot of $f_{\mathcal{EE}}(t)$ may correspond to a logarithmic correction. Figure 5(c) shows such a fit with $f_{\mathcal{EE}}(t) \sim (\ln t)^{\phi}$ with $\phi \simeq 0.80$. From the value of the above exponent $1/z\nu = 0.4624(29)$ we obtain $1/\nu = 1.0019(72)$ using $z_{mixed} = 2.1668(19)$. This estimate compares quite well with that obtained from $M(t)$, $E(t)$, and $f_{\mathcal{MM}}(t)$.

For $q=3$, in contrast to the Ising ($q=2$) case, both moments $f_{\mathcal{ME}}(t)$ and $f_{\mathcal{EE}}(t)$ exhibit asymptotic power-law behavior. The average slopes obtained from Figs. 5(a) and 5(b) are given by $1/z\nu = 0.5515(61)$ and $(2-\nu d)/z\nu = 0.1911(72)$. These values yield the static and dynamic exponents $1/\nu = 1.210(58)$ and $z = 2.193(129)$. It is interesting to see that this dynamic exponent is larger than $z_{mixed} = 2.173(2)$ given in (14) and is rather closer to those given in (10). However, one should also note that the error bars are much larger in this case.

One can therefore conclude that for the present system using the relaxation of the order parameter and the energy combined with the value of z_{mixed} yields better estimates for static exponents than using the second-order moments involving the energy fluctuations. From this point of view, the moments $f_{\mathcal{ME}}(t)$ and $f_{\mathcal{EE}}(t)$ may be used to check the consistency of the results obtained using the energy relaxation itself.

D. Short-time critical dynamics

At this point, for comparison, it is worthwhile to briefly describe the method using the short-time critical dynamics which offers an alternative way of determining the static and dynamic exponents. More details can be found in [4]. When quenched to T_c from the initial disordered state, but with sufficiently small "magnetization" M_0, the system exhibits a nonequilibrium scaling regime in which the order parameter typically shows an anomalous power-law increase as [5]

$$M(t) \sim M_0 t^{\theta} \tag{16}$$

before eventually relaxing toward its equilibrium value, where the exponent θ is a new nonequilibrium critical exponent. Though it typically takes a positive value, it becomes negative for some systems such as the tricritical system [38], the Ashkin-Teller model [39], the Blume-Capel model [40], the four-state Potts model [41], and the Baxter-Wu (BW) model [34,35,42]. The time scale τ_M associated with the power-law increase depends upon the magnitude of the initial magnetization as $\tau_M \sim M_0^{-z/x_0}$ where the scaling dimension x_0 is related to the other exponents as $x_0 = \theta z + \beta\nu$.

In practice, θ was obtained by linearly extrapolating the effective exponents θ_{eff} (for finite M_0) vs M_0 to $M_0 = 0$. Al-

ternative way of obtaining θ was first proposed by Huse [6]. Using a scaling ansatz for the nonequilibrium structure factor of the two-dimensional kinetic Ising model, Huse has shown that the autocorrelation function of the global order-parameter $\mathcal{M}(t)$ with random initial conditions exhibits a power-law behavior

$$\mathcal{A}_{\mathcal{M}}(t) = \frac{1}{N}\langle \mathcal{M}(t)\mathcal{M}(0)\rangle \sim t^{\theta}. \tag{17}$$

Huse has also shown that the spin autocorrelation function $A(t)$ exhibits a critical decay in time as

$$A(t) \equiv \frac{q}{q-1}\frac{1}{N}\left\langle \sum_i \left(\delta(\sigma_i(0),\sigma_i(t)) - \frac{1}{q} \right) \right\rangle \sim t^{-\lambda} \equiv t^{-d/z+\theta}. \tag{18}$$

Tomé and Oliveira [43] have proved that (18) holds for equilibrium as well as nonequilibrium systems (i.e., without detailed balance) possessing the global up-down symmetry. Later on, Tomé [44] showed that the validity of (18) is extended to systems with other symmetries. It is much more convenient to measure θ by measuring the autocorrelation $\mathcal{A}_{\mathcal{M}}(t)$ since one is free from cumbersome preparation of the initial states with very small magnetization and an extrapolation procedure to vanishing initial magnetization.

The new nonequilibrium exponent θ has been obtained as follows. For $q=2$, $\theta=0.191(1)$ (heat bath) and $\theta=0.197(1)$ (Metropolis) using (16) [4,23–25] and $\theta=0.19$ using (17) [6]. In addition, Grassberger [45] also measured the exponent θ as $\theta=0.191(3)$ using a damage-spreading method. Likewise, for $q=3$, the exponent θ takes the following values: $\theta=0.075(3)$ (heat bath) and $\theta=0.070(2)$ (Metropolis) using (16) [4,23–25] and $\theta=0.072(1)$ using (17) [41]. The exponent θ was also measured using (17) as $\theta=0.093(4)$ [46] for a nonequilibrium cellular automaton model with C_{3v} symmetry which belongs to the three-state Potts universality class [47]. In addition, there exists measured value of θ for $q=4$ using both (16) and (17), which are given, respectively, by $\theta=-0.0471(33)$ and $\theta=-0.0429(11)$ [41]. It is an interesting fact that the four-state Potts model and the BW model, which belong to the same static universality class, do not share the same nonequilibrium exponent θ: $\theta=-0.185(2)$ [42] or $-0.186(2)$ [35] for the BW model. It would be interesting as well to clarify the question as to whether this nonuniversal dynamic behavior is extended to the case of z in both systems.

Independent measurements of the exponents θ and λ using (17) and (18) provide an alternative way [4,20,23] of obtaining z through the relation $z=d/(\lambda+\theta)$. The measured values of λ and hence z are given by $\lambda=0.737(1)$ and $z=2.155(3)$ for $q=2$ and $\lambda=0.836(2)$ and $z=2.196(8)$ for $q=3$ [4]. As for the BW model, $\lambda=1.188(10)$ and $z=1.994(24)$ [42] were obtained using the continuous-time Monte Carlo algorithm. One disadvantage of this method is that the rather large value of λ induces strong fluctuations in its measurement, which is the main source of the error for the estimate of z.

With z in hand, one can use (11) with disordered initial states to obtain the ratio β/ν, or equivalently, the exponent $\eta \equiv 2\beta/\nu$ (for $d=2$). In order to determine β and ν separately, one can use the following scaling ansatz for the order parameter near and below T_c:

$$M(t,\epsilon) = t^{-\beta/z\nu}\mathcal{F}(t^{1/z\nu}\epsilon), \tag{19}$$

where $\mathcal{F}$ is the scaling function and ϵ is the reduced temperature defined as $\epsilon \equiv (T_c - T)/T_c$. Equation (19) reduces to (4) for $\epsilon=0$. Then one can give an estimate for $1/\nu$ using

$$\frac{\partial}{\partial \epsilon}\ln M\,(t,\epsilon)\big|_{\epsilon=0} = t^{1/z\nu}\left(\frac{d}{dx}\ln \mathcal{F}(x)\right)_{\epsilon=0}. \tag{20}$$

This method gives $1/\nu=1.03(2)$ (square lattice) [4] and $1/\nu=1.027(6)$ (triangular lattice) [25] for $q=2$ and $1/\nu=1.24(3)$ (square lattice) [4,21] and $1/\nu=1.223(8)$ (triangular lattice) [25] for $q=3$. But involving the difference of the order parameter at several close temperatures near T_c may cause considerable error in the estimate of the exponent ν. Our method (presented in Sec. III C) utilizing the energy relaxation can provide an alternative and better way of estimating the exponent ν without using (20).

IV. SUMMARY AND CONCLUDING REMARKS

Through Monte Carlo simulations we have investigated the nonequilibrium critical dynamics of the ferromagnetic q-state Potts model on a square lattice. The primary purpose of the present work was to evaluate the accuracy of the estimates the NER method can provide for both static and dynamic exponents of statistical systems. The ferromagnetic Potts model is an ideal test system for that purpose since the static critical properties of the model are exactly known.

In contrast to other nonequilibrium approaches, we utilized both the order parameter and energy relaxation. The ratio of the power-law exponents of the order parameter and the energy involves solely the static exponents. In order to separately measure the two independent static exponents, one first measures the dynamic exponent z by considering the order-parameter moments starting from either random or fully ordered initial states. It is found that in the present model, when the fully ordered initial states are employed, the time scale associated with the asymptotic scaling for which the relaxation of the second moments of the order parameter sets in seems to be much longer for higher q than that for the disordered initial states and may exceed the present simulation time window. As a result, the slopes obtained from the second moments of the order parameter may differ. One thus has to be very careful in obtaining the dynamic exponent z from the time-dependent moments for the order parameter. Once z is determined, the two independent exponents ν and β can be determined from the relaxation of the energy and the order parameter, respectively.

The present work has demonstrated that, in the case of the $q=2$ (Ising) model, this method can provide accurate estimates for the static and dynamic exponents provided that, as mentioned above, special care is taken in the choice of the initial states for the estimation of the dynamic exponent z. For example, the dynamic exponent z_{mixed} obtained from the relaxation of the second moment of the order parameter with

disordered initial states is more consistent with the relaxation of the order parameter and excess energy when exact values of the static exponents are assumed. In the case of the $q=3$ Potts model, even though the static exponents obtained with the same methods are less accurate than in the case of $q=2$, they still show reasonable agreement with the exact known values of the static exponents.

The fact that the dynamic exponent z does not appear in the ratio of the power-law exponents of the order parameter and energy may be used to clarify the nature of the phase transition whose critical properties are under debate. An outstanding example is the phase transition associated with the chirality order in the FFXY models. The relaxations of the order parameter and energy are expected to become slower for frustrated systems. Hence the above ratio can be measured with higher accuracy. We therefore tend to believe that once the critical temperature is accurately determined, the critical relaxations of the order parameter and energy for the chirality phase transition can tell whether the phase transition belongs to the Ising universality class or to the three-state Potts class, or else to an entirely different universality class.

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APPENDIX: CRITICAL RELAXATIONS OF MOMENTS OF THE ORDER PARAMETER AND ENERGY

The critical relaxations of the order parameter and energy and their higher moments can be obtained from the following scaling behavior of the nonequilibrium generating function $\psi(\epsilon,h,t)$ which reduces to the equilibrium free energy density in the limit $t\to\infty$:

$$\psi(\epsilon,h,t) = b^{-d}\tilde{\psi}(\epsilon b^{y_T}, h b^{y_h}, t b^{-z}) = t^{-d/z}\tilde{\psi}(\epsilon t^{y_T/z}, h t^{y_h/z}, 1), \tag{A1}$$

where b is the scaling factor, $\epsilon \equiv |T_c - T|/T_c$ the reduced temperature difference, and h the external (magnetic) field coupled to the order parameter. The above result was first derived by Suzuki [48]. In (A1), y_T and y_h are the scaling dimensions associated, respectively, with temperature and external field, which are given by $y_T = 1/\nu$ and $y_h = d - \beta/\nu$. The relaxation of the order parameter $M(t)$ at T_c is obtained by differentiating the generating function $\psi(\epsilon,h,t)$ with respect to the magnetic field h:

$$M(t) = \left(\frac{\partial\psi}{\partial h}\right)_{\epsilon=h=0} \sim t^{(y_h-d)/z} = t^{-\beta/z\nu}. \tag{A2}$$

Likewise, the energy relaxation is obtained from the derivative of the generating function with respect to the reduced temperature ϵ:

$$(E(t) - E_c) = \left(\frac{\partial\psi}{\partial\epsilon}\right)_{\epsilon=h=0} \sim t^{(y_T-d)/z} = t^{-(\nu d-1)/\nu z} = t^{-(1-\alpha)/z\nu}, \tag{A3}$$

where the hyperscaling relation $2-\alpha=\nu d$ was used in the last equality. Equations (A2) and (A3) give the leading order part of (4).

The second-order moment of the order parameter is accordingly obtained by differentiating twice $\psi(\epsilon,h,t)$ with respect to h:

$$\langle[\delta\mathcal{M}(t)]^2\rangle = \langle\mathcal{M}^2(t)\rangle - M^2(t) = \left(\frac{\partial^2\psi}{\partial h^2}\right)_{\epsilon=h=0} \sim t^{(2y_h-d)/z} = t^{(d-2\beta/\nu)/z}. \tag{A4}$$

Equation (A4) gives (11).

Likewise, the second-order moment of the energy is given by

$$\langle[\delta\mathcal{E}(t)]^2\rangle = \left(\frac{\partial^2\psi}{\partial\epsilon^2}\right)_{\epsilon=h=0} \sim t^{(2y_T-d)/z} = t^{(2-\nu d)/z\nu} = t^{\alpha/z\nu}. \tag{A5}$$

Equation (A5) gives the last member of (15).

Finally, the cross moment of the order parameter and energy is given by

$$\langle\delta\mathcal{M}(t)\,\delta\mathcal{E}(t)\rangle = \left(\frac{\partial^2\psi}{\partial\epsilon\,\partial h}\right)_{\epsilon=h=0} \sim t^{(y_T+y_h-d)/z} = t^{(1-\beta)/z\nu}. \tag{A6}$$

Dividing $\langle\delta\mathcal{M}(t)\,\delta\mathcal{E}(t)\rangle$ by $M(t)$ gives

$$\frac{\langle\delta\mathcal{M}(t)\,\delta\mathcal{E}(t)\rangle}{M(t)} \sim t^{1/z\nu}. \tag{A7}$$

Equation (A7) yields the first member of (15).

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