Scaling behavior beyond the Kibble-Zurek mechanism in driving critical dynamics

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We study the effects induced by the initial conditions in the driving critical dynamics. A protocol is proposed in which a system starts with a nonequilibrium initial state near the critical point. This driving critical dynamics is remarkably different from the dynamics described by the usual adiabatic–impulse–adiabatic scenario of the Kibble-Zurek mechanism. Instead, it is described by a universal relaxation–finite-time scaling–adiabatic scenario. The distinctive feature is the appearance of the relaxation stage in which the increment of the correlation time dominates and the external driving acts only as a perturbation. A unified scaling theory, which includes the initial scaling variables, is proposed to describe the scaling behaviors. The results are confirmed by numerical simulations of the two-dimensional Ising model.

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The Kibble-Zurek mechanism (KZM) [1–4] is a theory describing the driving critical dynamics in a variety of systems, ranging from classical phase transitions [5–19] to quantum phase transitions [20–31]. This mechanism is first proposed by Kibble in cosmological physics [1, 2]. Then, Zurek brought this proposal to condensed matter physics [3, 4]. Upon starting in temperature $T_0$, which is far away from the critical point $T_c$ and linearly changing $T$ at a given temporal rate $R$, the KZM divides the driving process into three stages. Among them, two adiabatic stages sandwich an impulse stage, in which the evolution is governed, according to the theory of finite-time scaling (FTS) [32, 33], by a constant time scale $\zeta_d \sim R^{-\nu z/\nu}$ that is shorter than the reaction time $\zeta_r \sim |\tau|^{-\nu z}$ and is thus out of equilibrium, where $\tau = (T - T_c)/T_c$, $r_T = z + 1/\nu$, and $\nu$ and $z$ are the critical exponents. The two time scales match at the boundaries, thus resulting in the scaling of the topological defect density predicted by the KZM. This scaling agrees with many numerical simulations and experiments [5–19]. Besides the topological defects, other quantities have also been shown to exhibit scaling behavior depending on the driving rate [32–35]. Furthermore, various other protocols have been proposed to generalize KZM to different kinds of driving [36].

Two prerequisites of the initial conditions are implicitly assumed in the original KZM [1–19]. One is that the initial state must be an equilibrium state, the other is that the initial distance to the critical point must be sufficiently large. However, these prerequisites need to be controlled and cross-checked carefully in experiments and numerical simulations [37]. This inspires systematical studies on the effects induced by the initial conditions. In quantum phase transitions, relevant studies have been reported [38–41] and the restrictive initial distributions that ensure the scaling of KZM have been identified [41]. However, up to now, the effects of the initial conditions on the KZM have been ignored in classical phase transitions [1–19, 36].

In this paper, we study the effects induced by the initial conditions in classical driving dynamics. For large $|\tau_0|$, this issue seems to be trivial, since the dissipative nature of the thermal dynamics makes any initial state decay to the equilibrium state in a microscopic time [42, 43]. Therefore, the initial condition is irrelevant and the evolution is identical to the case that starts with the equilibrium state. In contrast, when the initial distance to the critical point is small, the initial information can be remembered for a macroscopic time owing to the critical slowing down [44]. In particular, the relaxation starting with a small magnetization $M_0$ and a van-
ishing correlation length exhibits an initial slip during which \( M \sim M_0 t^\theta \) with \( \theta \) a new critical slip exponent (see the red dashed curve in Fig. 1(a)). This results from the increases with time of the correlation length, \( \xi \sim t^{1/\nu} \) and the correlation time \( \zeta \sim t^z \sim t \). When this nonequilibrium initial condition is combined with the external driving, Fig. 1(a) shows that the dynamics is significantly changed by the initial condition. Thus it is natural to ask how the usual adiabatic–impulse–adiabatic scenario of the KZM is changed by the initial condition.

To answer this question, we explore a protocol of the driving dynamics starting with an uncorrelated nonequilibrium initial state near the critical point. A relaxation–FTS–adiabatic scenario, as sketched in Fig. 1(b), is proposed to characterize this kind of driving dynamics. This can be understood as follows. Since the dissipative nature of the dynamics [42, 43], after a microscopic time the universal behavior, which is controlled by the low-energy modes, emerges. In general, in the universal stage, the critical dynamics is dominated by the shortest relevant time scale near the critical point. For the present protocol, there are three possible relevant time scales, which are the equilibrium correlation time scale \( \zeta_e \), the external-driving-induced finite time scale \( \zeta_d \) [32, 33], and the time scale \( \zeta_t \) characterising the initial relaxation [45, 46]. It is their possible competition that gives rise to various regimes. As \( \zeta_t \) increases from zero [45, 46] and is smaller than both the potential \( \zeta_e \) and \( \zeta_t \), a relaxation dynamics dominates the universal stage after the microscopic time. We call this stage the relaxation stage, in which the external driving is only a perturbation. Yet, the driving then takes over and differentiates the evolution from the pure relaxation in the absence of the driving as can be seen from the dashed and solid curves in Fig. 1(a). The FTS stage and finally the adiabatic stage then follow in which the relevant time scales are \( \zeta_d \) and \( \zeta_t \), respectively. This then shows that the adiabatic–impulse–adiabatic scenario of the KZM [1–4] alone cannot describe the whole driving process as it has not taken the initial conditions into account.

To confirm quantitatively the present relaxation–FTS–adiabatic scenario, in the following, a scaling theory is proposed, which includes the initial distance to the critical point and the initial order parameter. According to this theory, the scaling behaviors in different stages are obtained. In particular, in the relaxation stage, we show that the external driving brings a universal power-law deviation from the pure relaxation dynamics. Aside from changing \( \tau \), the scaling behavior for changing a symmetry-breaking field \( b \) is also considered. The results show the universality of the present scenario and the scaling theory including the initial conditions. These conclusions are confirmed by the numerical results of the two-dimensional (2D) Ising model.

Near the critical point, the scaling behaviors of macroscopic quantities can be readily described by a scale transformation. For the order parameter \( M \), we propose that the rescaling of a factor \( b \) results

\[
M(t, R, M_0, \tau_0, \tau) = b^{-\beta/\nu} M\left(t b^{-z}, R b^{\nu/\nu z}, U(M_0, b), \tau_0 b^{1/\nu}, \tau b^{1/\nu}\right),
\]

where \( |\tau_0| \ll 1 \), and \( \beta \) is the critical exponent defined as \( M \propto |\tau|^\beta \) in the ordered phase in equilibrium, and \( U(M_0, b) \) is the universal characteristic function describing the rescaled initial magnetization [47]. For a small \( M_0 \), \( U(M_0, b) = M_0 b^{\nu z} \) with \( x_0 \) being the scaling dimension of \( M_0 \) [45, 46]. This indicates that \( M_0 = 0 \) is a fixed point since \( U(0, b) = 0 \) for arbitrary \( b \geq 1 \). For a hard-spin system, in which the order parameter is bounded, the saturated \( M_0 \) is another fixed point, since the rescaled \( M_0 \) is invariant under coarse graining [47]. Compared with the scaling transformation of driving dynamics starting with an equilibrium state, two additional scaling variables, \( \tau_0 \) and \( M_0 \), are included in Eq. (1). However, they appear only for small \( |\tau_0| \); for large \( |\tau_0| \), they do not appear. Note that the scaling behavior of \( R \) is independent of \( \tau_0 \) and \( M_0 \). \( R \) always contributes an effective time scale \( \zeta_d \sim R^{1/z} \) regardless of the initial conditions. Equation (1) with a small \( M_0 \) can be justified by a renormalization-group theory which combines the short time critical dynamics [45, 46] and the FTS theory [32, 33].

The scaling forms of different stages can be obtained from Eq. (1) by comparing the relevant time scales. The first stage, in which \( t \) is small, the correlation time \( \zeta_t \) is small and increasing. As a result, the relaxation dynamics dominates. By setting \( t b^{-z} = 1 \), we arrive at the scaling form

\[
M(t, R, M_0, \tau_0) = t^{-\beta/\nu z} f_1(R t^{\nu z/\nu}, U(M_0, t^{1/z}), \tau_0 t^{1/\nu}),
\]

where \( f_1 \) is a scaling function. Detailed scaling behaviors can be obtained from Eq. (2) as follows.

For \( \tau_0 = 0 \) and a small \( M_0 \), \( U(M_0, t^{1/z}) = M_0 t^{x_0 z/\nu} \). One can expand \( f_1 \) in \( R t^{\nu z/\nu} \) and \( M_0 t^{x_0 z/\nu} \) to the second order, and thus obtains

\[
M \simeq M_0 t^\theta f_1'(0, 0, 0) + t^\theta + R M_0 f_1''(0, 0, 0),
\]

where \( \theta = (x_0 - \beta/\nu) / z \) and a prime stands for a partial derivative. In Eq. (3), the first term describes the usual critical initial slip in which the magnetization increases with time [45, 46]. The reason is that in the early stage, for the vanishing initial correlation, the system exhibits a mean-field phase ordering process as the real critical point is below its mean-field value. The second term of Eq. (3) displays the external-driving-induced deviation from the critical initial slip. It is a cross term between \( M_0 \) and \( R \) and arises from the fact that, if \( M_0 = 0 \), \( M \) remains zero as \( \tau \) does not break the symmetry. The external driving, which dominates near the critical point in the ordinary KZM, here acts only as a perturbation.

For \( \tau_0 = 0 \) and the saturated \( M_0 \), \( U(M_0, t^{1/z}) = M_0 \). In the initial stage, the order parameter \( M \) now decays according to

\[
M \simeq t^{-\beta/\nu z} f_1(0, M_0, 0) + R t^{(\nu z - \beta)/\nu z} f_1'(0, M_0, 0),
\]
where the first term is the relaxation dynamics [48] and the second term is again the perturbation induced by the external driving. Note that for $R > 0$, $f_1(0, M_0, 0) < 0$ because $M$ must decrease as the temperature increases.

According to Eq. (2), the crossover between the relaxation and the FTS regimes occurs at $R^n R^{f 2 / z} \sim 1$, i.e., $t \sim R^{- z / n R^{f}}$. This is reasonable as it is the driving time $c_n$ and thus coincides with the frozen instant which is the crossover between the adiabatic and impulse regimes of the KZM. However, as displayed in Fig. 1, the scaling function is significantly changed by the initial condition. With the scale transformation (1), we obtain the scaling form by setting $R^n R^{f} = 1$,

$$M(R, M_0, \tau) = R^{\beta / n R^{f}} f_2(t_0 R^{- 1 / n R^{f}}, U(M_0, R^{- 1 / n R^{f}}), R^{\gamma R^{- 1 / n R^{f}}}).$$ (5)

For small $M_0$, $U(M_0, R^{- 1 / n R^{f}}) = M_0 R^{- x_0 / n R^{f}}$, while for the saturated $M_0$, $U(M_0, R^{- 1 / n R^{f}}) = M_0$. For $\tau = 0$, when the driving dynamics starts with the saturated $M_0$, Eq. (5) is quite similar to the usual scaling form of KZM [32, 33], although the scaling functions are different, because they characterize different evolutions with distinct initial conditions. In addition, we note that in the original KZM, only the impulse region is out of equilibrium as it is the FTS region [29, 32, 33]. However, here both the relaxation stage and the FTS stage are nonequilibrium albeit due to different reasons, viz., the first arises from the initial conditions whereas the second from the driving.

When $\tau > R^{\beta / n R^{f}}$, the system enters the adiabatic stage, in which $c_0 < c_n$, and the scaling form is

$$M(R, M_0, \tau) = \tau^\beta f_3(0, U(M_0, R^{\gamma R^{- 1 / n R^{f}}}, R^{\gamma R^{- 1 / n R^{f}}})$$ (6)

Note that the crossover to this adiabatic stage is similar to the usual impulse-adiabatic crossover in KZM. This is confirmed in Fig. 1, in which the place at which the curve of the usual KZM tends to zero is close to the corresponding place of the curve starting with a nonequilibrium inital condition.

The inclusion of the nonequilibrium initial conditions in the scale transformation is universal for varying other variables. For example, consider the situation of changing the symmetry-breaking field $h$ as $h = h_0 + R h t$ with a small $h_0$. For simplicity, $\tau$ is fixed to 0. In this situation, there are also three stages in the driving process.

In relaxation region, the scaling form for small $M_0$ is

$$M(t, R h, M_0, h_0) = W^{- \beta / n z} f_1(R h t^{\beta R^{f} / z}, M_0 t^{\beta R^{f} / z}, h_0 t^{\beta R^{f} / n z}),$$ (7)

with $t^{\beta R^{f} / z} = z + \beta R^{f} / n z$, while in the FTS region, the scaling form changes to

$$M(R h, M_0, h_0) = W^{- \beta R^{f} / n z} f_1(M_0 R^{- x_0 R^{f} / n z}, h_0 R^{- \beta R^{f} / n z}, h R^{- \beta R^{f} / n z}).$$ (8)

Similar to the discussion of Eq. (5), when we start with $h_0 = 0$ and the saturated $M_0$, Eq. (8) appears to coincide with the FTS scaling form starting in the adiabatic stage [32, 33]. However, the scaling function is different. We note that this situation has been considered in Ref. [49], where a method to determine the critical exponents is proposed. However, the relaxation dynamics is not discussed there.

To confirm the scaling theory, we take the 2D classical Ising model as an example. Its Hamiltonian is

$$H = - \sum_{<i,j>} S_i S_j + h \sum_i S_i,$$ (9)

where $S_i = \pm 1$. The critical point for the model (9) is $T_c = 2 / (\log(\sqrt{2} + 1)) [50]$. The exponents are $\beta = 1 / 8$, $\nu = 1$, $\delta = 15$ [50], $\gamma = 2.1667$ [42] and $\theta = 0.191 [51–53]$. These will be taken as inputs to verify the scaling forms. The single-spin Metropolis algorithm [54] is used. We choose a lattice size of 5000, which has been checked to produce a negligible size effect. Periodic boundary conditions are applied throughout. Typically, we calculated averages over between 2000 and 3000 samples, which guarantee that the relative errors are smaller than 1%.

First, we verify the scaling theory by classifying the stages of the evolution and examining the scaling form (5). Figure 2(a) shows the dependence of the order parameter $M$ on $\tau$ with different initial magnetization $M_0$ for $\tau_0 = 0$. When $\tau$ is small, $M$ increases with $\tau$ and thus both $R$ and $\tau$ in the initial stage. This is similar to the critical initial slip in the pure relaxation dynamics and is thus the relaxation stage. When $\tau$ becomes larger, $M$ decreases as $\tau$ increases. In this stage, $M$ increases with $R$ and the curves of evolution show hysteresis. This is the typical behavior of FTS stage [32, 33]. Then follows the adiabatic stage, in which $M$ is zero, independent of the initial condition and the driving rate. Because $M_0$ has been chosen in such a way that $M_0 R^{- x_0 R^{f} / n R^{f}}$ is fixed, the curves collapse onto each other after rescaling, confirming that $M_0$ is an indispensable scaling variable.

Second, Fig. 2(b) shows the dependence of the order parameter $M$ on $\tau$ with different initial magnetization $M_0$ for $\tau_0 \neq 0$. For fixed $M_0 R^{- x_0 R^{f} / n R^{f}}$ and $M_0 R^{- 1 / n R^{f}}$, the rescaled curves collapse well onto each other. This confirms that $\tau_0$ is also a scaling variable. In Fig. 2(b), the three stages are also demonstrated. In the relaxation stage, the order parameter also increases with $\tau$, then crosses over to the FTS stage, in which $M$ increases with $R$.

Third, we study the effects of the external driving according to Eqs. (3) and (4). In Fig. 3(a), the difference between the driving relaxation and pure relaxation dynamics satisfies a power-law relation, $|M - M_0 f_1(0, 0, 0)| \sim t^{\beta R^{f} / n R^{f} / z}$, according to Eq. (3). The fitting result gives $\beta R^{f} / n R^{f} / z = 1.696(2)$. This agrees with the theoretical value of $\beta R^{f} / n R^{f} / z = 1.652$ with a deviation of about 2%. For the case of the saturated $M_0$, which is $M_0 = 1$ for Ising model, as shown in Fig. 3(b), $|M - M_0 f_1(0, 1, 0)|$ changes with $t$ with an exponent $1.499(4)$, which is close to $\beta R^{f} / n R^{f} / z = 1.403$, consistent with Eq. (4). The deviations should arise from the contributions of higher order terms in the expansions.

Fourth, Fig. 4 shows the results of changing $h$ as $h = h_0 - R h t$ with some small and negative $h_0$. Three stages also show manifestly similar to those in Fig. 2. The rescaled curves
with different $R_h$ and $M_0$ collapse well onto each other for fixed $M_0 R_h^{\nu \eta / \nu_T}$ and $|h_0| R_h^{\nu \eta / \nu_T}$. This confirms both that the scaling form must include $h_0$ and $R_h$ as the scaling variables as shown in Eq. (8) and that the relaxation–FTS–adiabatic scenario is generally applicable in the driving dynamics starting with a nonequilibrium state near the critical point.

Previous studies show that the usual KZM can be generalized to the quantum phase transitions [20–31]. The present scaling theory, however, cannot be generalized to the real-time dynamics of the quantum phase transitions. The reason is that the emergence of the universal dynamics results from the dissipative nature of the thermal dynamics. For the quantum situation on the other hand, the high-energy modes cannot decay because of the unitary nature of the dynamics. It has been shown that for the real-time quantum relaxation, there is no similar critical initial slip behavior [55]. However, for the imaginary-time relaxation, the scaling behavior is similar to the classical case [55, 56]. Accordingly, for the imaginary-time driving, we have checked that the scale transformation (1) can indeed describe the evolution of the order parameter.

In summary, we have systematically studied the driving dynamics starting with a nonequilibrium initial state near the critical point. We have found that the well-known adiabatic–impulse–adiabatic scenario of the KZM has to be modified to the relaxation–FTS–adiabatic scenarios. A scaling theory has been suggested to characterize the scaling behavior. The initial conditions, including the initial distance to the critical point and the initial order parameter, have to be included in this theory. Besides the adiabatic stage and the external-driving-dominated FTS region, there exists a relaxation regime in the short time stage, in which the relaxation dynamics dominates and the external driving acts only as a perturbation. The scaling behavior in this stage is remarkably different from the dynamics of KZM. These results have been confirmed by numerical results of the Ising model. In addition, while the present scaling theory cannot be generalized to the real-time dynamic quantum criticality, it can apply to the imaginary-time one. This poses a question as to what extent scaling behavior shares in both classical and quantum phase transitions.

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