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Kibble-Zurek mechanism and infinitely slow annealing through critical points

Giulio Biroli,[1] Leticia F. Cugliandolo,[2] and Alberto Sicilia[3]
[1]*CEA, Institut de Physique Théorique (IPhT) URA 2306, F-91191 Gif-sur-Yvette, France*
[2]*LPTHE UMR 7589, Université Pierre et Marie Curie–Paris VI, 4 Place Jussieu, 75252 Paris Cedex 05, France*
[3]*Department of Chemistry, University of Cambridge, Lensfield Road, CB2 1EW Cambridge, United Kingdom*
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We revisit the Kibble-Zurek mechanism by analyzing the dynamics of phase ordering systems during an infinitely slow annealing across a second-order phase transition. We elucidate the time and cooling rate dependence of the typical growing length, and we use it to predict the number of topological defects left over in the symmetry broken phase as a function of time, both close and far from the critical region. Our results extend the Kibble-Zurek mechanism and reveal its limitations.

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The out-of-equilibrium dynamics induced by a quench are the focus of intense research [1,2]. Interesting realizations are quenches through a second-order phase transition, which take the system from the symmetric phase into the symmetry broken one. Below the transition, system-size dependent times are needed to reach equilibrium and to realize the spontaneous symmetry-breaking process. Before this (typically unreachable) asymptotic limit the symmetry is broken only locally: the system is formed by ordered regions of size growing with time [3]. Only when this size reaches the order of the volume of the sample the symmetry is broken globally and the spatial average of the order parameter deviates from zero. The majority of theoretical studies focused on the dynamics after infinitely rapid quenches although experimentally quenches are performed at finite speed. Indeed, since the typical time scale on which the system evolves is its age, i.e., the time elapsed since crossing the critical point, finite quench time scales (τ_Q) eventually become short compared to the relaxation time. Thus, they alter the out-of-equilibrium dynamics at short times only. The opposite limit of an extremely slow annealing, corresponding to very long τ_Q, needs a separate treatment. Surprisingly, this has not been studied in detail in the statistical physics literature with, however, some exceptions for disordered systems [4–6]. It has, instead, attracted a lot of attention within the cosmology and, more recently, the condensed-matter communities. An explanation of the slow dynamics induced by this protocol was given by the so-called Kibble-Zurek (KZ) mechanism [7–10]. This is an *equilibrium scaling argument* that yields an estimate for the density of topological defects left over in the ordered phase as a function of the quenching rate close to the critical point. The argument has been recently generalized to study very slow "quantum annealing" across quantum phase transitions in isolated systems [11–13].

The aim of this work is to obtain a more complete picture of the slow dynamics induced by an extremely slow annealing. With numerical and analytical arguments we unveil the limitations of the KZ approach, and we obtain a full scaling description of the slow dynamics. Our main result is that the dynamic evolution is characterized by a first adiabatic regime in agreement with KZ, followed by critical coarsening and, finally, standard coarsening at very long times. We present a universal scaling function that characterizes the growth of the correlation length out of equilibrium under slow cooling procedures, and we relate it to the number of topological defects in cases in which these exist.

We start our discussion by recalling the KZ mechanism [8–10]. We take a system in equilibrium at equilibrium at a value $g_0 > g_c$ of the control parameter in the symmetric phase and subsequently anneal it at finite rate (in typical situations g corresponds to temperature). As KZ, we focus on the protocol $g(t)=g_c(1-t/\tau_Q)$ starting from, say, $g_0=g(-\tau_Q)=2g_c$. Henceforth we use the standard notation of dynamical critical phenomena [14] and we set the microscopic time and length scales to one. Far from the critical point the equilibrium relaxation time, τ_{eq}, is barely larger than the microscopic time. Thus, for very small annealing rate, i.e., very long τ_Q, the system evolves adiabatically and remains in equilibrium at the running $g(t)$. However, this regime must inevitably break down since τ_{eq} diverges at the critical point as $|\Delta g|^{-\nu z_{eq}}$ with $\Delta g \equiv g-g_c$. KZ argued that the end of the adiabatic regime occurs when the remaining time, $\hat{t}$, needed to reach g_c becomes smaller than τ_{eq}. This is certainly a lower bound and yields $\hat{t} \propto \tau_{eq}(\hat{g}) \propto \tau_Q^{\nu z_{eq}/(1+\nu z_{eq})}$ with $\hat{g}=g(-\hat{t})$. The distance from the critical point at $-\hat{t}$ is $\Delta\hat{g} \propto \tau_Q^{-1/(1+\nu z_{eq})}$. KZ assumed that after $-\hat{t}$ the topological defect configuration remains frozen, in the sense that the order parameter ceases to evolve. In this so-called "impulse" regime the effect of lowering g is to reduce fluctuations, which are in general of thermal origin since very often g is related to the temperature. The main prediction of KZ is the number of topological defects, N, at the symmetric instant $\hat{t}$ where the coupling-constant equals $g_c-\Delta\hat{g}$. Within their approach N is inherited from the configuration at $-\hat{t}$, it is therefore equal to the number of defects in equilibrium at $\hat{g}$, and it is estimated to be $N(\hat{t}) \simeq [f^2\xi_{eq}(\hat{g})]^{-d} \simeq f^{-2d}|\Delta\hat{g}|^{d\nu}$ with f of the order of 1. Knowing the τ_Q dependence of $\Delta\hat{g}$ allows one to derive the τ_Q dependence of N,

$$N(\hat{t}) \propto \tau_Q^{-d\nu/(1+\nu z_{eq})} \quad \text{at} \quad \hat{t} \propto \tau_Q^{\nu z_{eq}/(1+\nu z_{eq})}. \tag{1}$$

We stress that for each τ_Q this expression should be measured at the special instant $\hat{t}(\tau_Q)$ after the phase transition. The system's behavior at $t > \hat{t}$ is not fully addressed by KZ. In some publications it is assumed that any further evolution [15,16] can be neglected, whereas in others it is reckoned that after $\hat{t}$ the system resumes its out-of-equilibrium evolution with a mechanism that depends on the problem at hand (domain growth, vortex-antivortex diffusion and annihilation, etc.) [9] and the density of defects may therefore continue to decrease although no detailed study was performed. Numerous numerical [15–19] and experimental [20–24] papers tested the quantitative consequences of the Kibble-Zurek mechanism with variable results. While the numerical studies claimed that they successfully verified the predictions, the conclusions are less clear in the experimental works that studied vortex formation in superfluid ^{4}He and ^{3}He with null results in the former [20] and agreement with the KZ prediction in the latter [21]. See [22–24] for discussions of some recent experimental results disagreeing with the KZ prediction.

In the following we revisit the KZ scaling analysis. We focus on the dynamics of classical systems coupled to an environment, a setting in which the dynamics are stochastic and the energy, directly linked to the number of topological defects, is not conserved. We use the temperature of the thermal bath as the control parameter driving the second-order phase transition and a linear cooling rate $T(t)=T_c(1-t/\tau_Q)$. These choices are made to keep the discussion simple; extensions to more complicated protocols are straightforward and will be partially addressed later. Moreover, we restrict to systems with a unique equilibrium correlation length and a single dynamic counterpart, the typical growing length. We solely deal with problems with power-law scaling laws, which link, e.g., the correlation length to the distance from criticality, and length scales to time scales [25]. These restrictions exclude from the analysis complex systems with several competing lengths and problems with quenched disorder. Henceforth we focus on the growth law of the size of the correlated regions, $R(t)$. This will allow us to discuss systems characterized by topological defects as well as those that are not from the same point of view. We shall explain below how the density of topological defects can be obtained from $R(t)$.

Let us start our analysis with some simple remarks. First, although the initial adiabatic regime and the departure from it are expected, the existence of the impulse regime is questionable. During this regime, which would take place between $-\hat{t}$ and $\hat{t}$, the system is supposed not to evolve [7–10]. However, it is well known that after a rapid quench into the critical region any system undergoes *critical coarsening* described by the growth of a *typical linear length scale* for correlated regions, $R(\Delta t)\sim\Delta t^{1/z_{eq}}$ where Δt is the time spent in the critical region and z_{eq} is the exponent that links the equilibrium relaxation time and correlation length close to criticality [26,27]. Above criticality, the major difference between slow and rapid quenches is in the extension of the adiabatic regime. The slower the quench or the annealing, the closer the system gets to the critical point in equilibrium. However, also for very slow annealing, the system eventually departs from the adiabatic evolution and has to undergo critical coarsening.

Our second remark is that once getting across the critical point, when the running temperature $T(t)$ is far enough from T_c, the dynamics crosses over to standard coarsening. In order to get a better insight into this process, let us recall that an infinitely rapid quench to a temperature $T<T_c$ leads to a growth law $R\simeq\lambda(T)\Delta t^{1/z_d}$ [1]. Now z_d is the *dynamic exponent* that, quite generally, is different from z_{eq} and depends on the dynamic rules. The prefactor vanishes at T_c and is characterized by a singular power law $\lambda(T)\simeq|T-T_c|^{\nu(-1+z_{eq}/z_d)}=\xi_{eq}^{1-z_{eq}/z_d}$ [28]. If the annealing rate is finite, one naturally expects the growth law at long times and far from the critical point to be $R\simeq\lambda(T(t))\Delta t^{1/z_d}$. The reason is that the dynamical process renormalizing the value of $\lambda(T(t))$ should be finite and, hence, evolve on a much faster timescale than the coarsening one which instead is of the order of the age of the system and diverges with t.

We now endeavor to connect the dots and present a general scenario for infinitely slow annealing. Our main conjecture, which is motivated by the previous discussion and the fact that the system stays for a very long time in the vicinity of the critical point, involves the growth of the length scale $R(t)$,

$$R(t)\simeq\xi_{eq}[T(t)]f\left\{\frac{t}{\tau_{eq}[T(t)]}\right\}. \tag{2}$$

This asymptotic form encompasses equilibrium above the critical point, $x\equiv t/\tau_{eq}[T(t)]\ll-1$, critical coarsening, $x\propto O(1)$, and the crossover to standard coarsening $x\gg1$. The limits of $f(x)$ are obtained by requiring to find the expected adiabatic behavior and standard coarsening on the two extremes,

$$R(t)\simeq\begin{cases}\xi_{eq}(T(t)) & t\ll-\tau_{eq}(T(t))\\ [\xi_{eq}(T(t))]^{1-(z_{eq}/z_d)}t^{1/z_d} & t\gg\tau_{eq}(T(t))\end{cases}. \tag{3}$$

This imposes that $f(x)$ be a constant for $x\ll-1$ and proportional to x^{1/z_d} for $x\gg1$. We expect the scaling function $f(x)$ to be universal since it describes evolution on diverging time and length scales close to the critical point. A sketch of ξ_{eq} and R is shown in Fig. 1. Our scaling assumption applies to coarsening with and without topological defects. In the former case, the *decaying typical number of topological defects*, $N(t)\simeq R(t)^{-d}$, reads for $t\gtrsim\tau_Q$,

$$N(t)\simeq\tau_Q^{d\nu/z_d(z_{eq}-z_d)}t^{-d/z_d[1+\nu(z_{eq}-z_d)]}. \tag{4}$$

Note that a qualitatively similar dependence on t and τ_Q was found numerically in [29] in a system with vortex-antivortex pairs. Evaluating the above expression at $t=\hat{t}=\tau_Q^{\nu z_{eq}/(1+\nu z_{eq})}$ we recover KZ's result [Eq. (1)]. Ours, however, is more general since it applies to any time t and it allows one to describe all the slow annealing evolution. For example, $N(t)\propto\tau_Q^{-d/z_d}$ on times of the order of the inverse annealing rate, $t\simeq\tau_Q$, thus showing that a substantial decrease takes place after $\hat{t}$. In comparison with the KZ mechanism, our arguments allow one to understand why $R(\hat{t})\simeq fR(-\hat{t})$ with a factor f that can be as large as 10 in some cases [15]. This was somewhat mysterious in the KZ scenario where defects are frozen out in the impulse regime. We understand the reduction in the number of topological defects as due to critical coarsening. Taking this phenomenon into account is crucial for more general annealing protocols, e.g., $T(t)=\theta(-t)T_c(1-t/\tau_Q^{(1)})+\theta(t)T_c(1-t/\tau_Q^{(2)})$. For a large ratio $\tau_Q^{(2)}/\tau_Q^{(1)}$ the system spends a long time in the critical region and $R(t)$ evolves

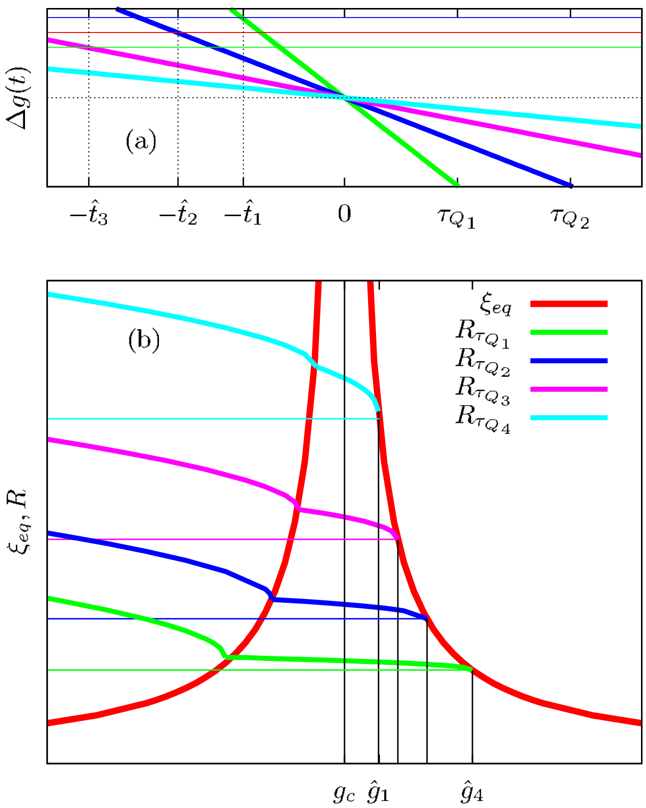

FIG. 1. (Color online) (a) The control parameter, $\Delta g(t)=[g(t)-g_c]/g_c$, for different cooling rates. The crossover between adiabatic and out of equilibrium dynamics are signaled as $-\hat{t}_i$ for $\tau_{Q_i}<\tau_{Q_{i+1}}$. (b) Sketch of the control parameter dependence of the equilibrium correlation length (thick red line) and the dynamic growing length R for four linear cooling rate procedures with $\tau_{Q_i}<\tau_{Q_{i+1}}$. Values of the control parameter at which the dependence changes from adiabatic to critical are shown as $\hat{g}_i$ (for simplicity we plot them as singular points in the evolution of R. In reality they just correspond to crossovers). For comparison the assumption of constancy during the impulse and subcritical regimes are shown with thin horizontal lines.

during the critical coarsening from $[\tau_Q^{(1)}]^{\nu/(1+\nu z_{eq})}$ to $[\tau_Q^{(2)}]^{\nu/(1+\nu z_{eq})}$.

In the following we provide numerical evidence for the conclusions outlined above by presenting results of a Monte Carlo simulation (using the heat bath algorithm with random sequential updates) of the $2d$ Ising model (IM) on square and triangular lattices. In particular, we check Eqs. (2)–(4) and the universality of the scaling function $f(x)$. We equilibrate the system at $T_0=2T_c$, and we use a linear cooling rate that takes the temperature of the bath from T_0 at $t=-\tau_Q$ to $T=0$ at $t=\tau_Q$. We find that the system undergoes an adiabatic evolution until it falls out of equilibrium close to T_c. The typical correlation length, $R(t)$, is extracted from the analysis of the space-time correlation $C(r,t)\equiv\langle s(\vec{x})s(\vec{x}+\vec{r})\rangle \simeq g[r/R(t)]$ with the average taken over 100 initial conditions and noise realizations. We use various ways to determine R and verify that they yield equivalent results. Two of them are $C[R(t),t]=1/2$ and $R(t)=\int d^2r r^{\zeta}C(r,t)/\int d^2r r^{\zeta-1}C(r,t)$ with ζ a parameter that is chosen for convenience, namely, to weigh differently shorter or longer distances. In the top panel of Fig. 2 we test the scaling hypothesis, Eq. (2), and the limits of the scaling function $f(x)$ [Eq. (3)]. For both the square and triangular lattices we find very good agreement between numerical data and theoretical expectation. The square-root growth at positive times demonstrates that standard coarsening cannot be ignored. The scaling collapse improves, as expected, restricting the range of $|x|$.

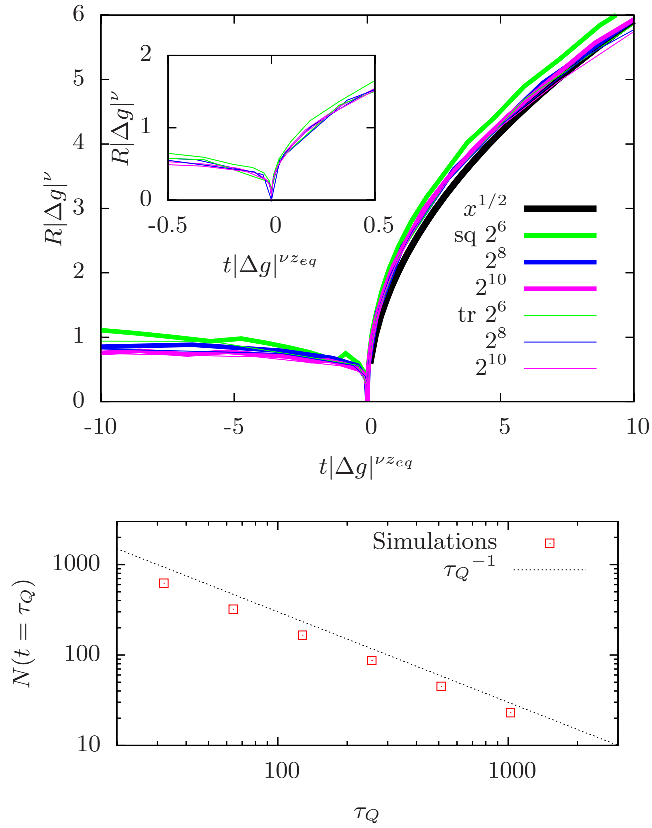

FIG. 2. (Color online) Top panel: Test of dynamic scaling hypothesis (2) and the limits [Eq. (3)] in the $2d$IM on a triangular and a square lattice, annealed at different cooling rates given in the key. A zoom on the critical region $|x|\lesssim 1$ is shown in the inset. The exponents are $\nu=1$, $z_{eq}=2.17$, and $z_d=2$. Bottom panel: number of defects at $t=t_Q$ for different cooling rates. Points represent the numerical data while the line corresponds to the prediction $N(\tau_Q)=\tau_Q^{-d/z_d}$

A zoom on the small $|x|$ region is shown in the inset. Moreover, we find that the scaling functions for square and triangular lattices coincide within numerical accuracy, confirming the universality of $f(x)$. The bottom panel of Fig. 2 displays $N(\tau_Q)$ and confirms the τ_Q^{-d/z_d} decay; the power is shown as a guide to the eyes next to the data.

A further test is provided by the analytic solution to the evolution of the $O(N)$ model in the large N limit for a very slow annealing. This is a $\lambda\phi^4$ field theory in which the order parameter is upgraded to an N-dimensional vector and the fourth-order term in the double-well potential is conveniently normalized to allow for an $N\to\infty$ limit in which the model becomes solvable but still nontrivial [1]. Note that although there are no topological defects, since the large N limit is taken at fixed dimension, $N\gg d$, the dynamics are still characterized by a growing correlation length $R(t)$. The analysis of a finite rate quench is a simple generalization of the treatment of infinite rate ones (see, e.g., [1]). We find that scaling (3) holds with $\nu=1/2$ and $z_d=z_{eq}=2$ in all $d>2$. Due to the coincidence of the z exponents the prefactor in the bottom expression of Eq. (3) equals one and the dependence on τ_Q disappears.

As a summary we analyzed the dynamic evolution induced by annealing with rate $1/\tau_Q(\tau_Q\to\infty)$ in pure systems characterized by conventional dynamic scaling and standard low-temperature coarsening. We obtained a complete picture of the dynamics which is characterized by three regimes: adiabatic, critical coarsening, and standard coarsening. Using scaling arguments we found the growth law of the correlation length during the annealing and its τ_Q scaling dependence. The crossover between adiabatic and coarsening regimes is governed by a universal scaling function. We tested our findings with numerical simulations of the $2d$ Ising model and a large N analysis of the $O(N)$ model in $d>2$. Our results generalize the KZ mechanism and, at the same time, show its limitation. In particular we find that the defect dynamics are not frozen in the so-called impulse regime as it can be found by using more general annealing protocols than a linear ramp in temperature.

Physical situations in which understanding the evolution during a slow annealing is important and which we plan to study in the future are disordered and quantum systems. Several studies have dealt with the former; see, e.g., [4–6]. The latter have only recently received attention in connection with quantum quenches and annealing in cold atoms. In these cases the conditions are different from the ones analyzed in this Rapid Communication since *isolated* systems in which a coupling is slowly changed through a quantum critical point are usually considered. The absence of the thermal bath may drastically change the physics. The KZ mechanism has been argued to apply *mutatis mutandis* to the isolated quantum case as well [11,12]. This has been verified in some integrable cases [13].

We close with a note on an exact study of the cooling rate effects in the relaxation of the classical Ising chain with Glauber dynamics by Krapivsky that shows qualitative but not quantitative agreement with the KZ mechanism [30].

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