Kibble-Zurek mechanism and infinitely slow annealing through critical points

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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, times scaling with the system size 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 the volume of the sample the symmetry is broken globally and for disordered systems [4–6]. It has, instead, attracted a lot of attention within the cosmology and, more recently, statistical physics literature with, however, some exceptions [7–10]. This generalized 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 a 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 find a new 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 a critical 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. From the critical point the equilibrium relaxation time, $\tau_{eq}$, is barely larger than the microscopic time. Thus, for very small annealing rate, i.e. very long $\tau_Q$, the system evolves adiabatically and remains in equilibrium at the running $g(t)$. However, this regime must inevitably break down since $\tau_{eq}$ diverges at the critical point as $|\Delta g|^{-\nu z\nu z c}$ 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 $\tau_{eq}$. This is certainly a lower bound and yields $\hat{t} \sim \tau_{eq}(\hat{g}) \sim \tau_Q^{-\nu z\nu z c/(1+\nu z\nu z c)}$ with $\hat{g} = g(\hat{t})$. The distance from the critical point at $\hat{t}$ is $\Delta g \propto \tau_Q^{-1/(1+\nu z\nu z c)}$. 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
We stress that for each $\tau_Q$ this expression should be measured at the special instant $\hat{t}(\tau_Q)$ after the phase transition. The system’s behaviour at $t > \hat{t}$ is not fully addressed by KZ. In some publications it is assumed that any further evolution 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-anti-vortex diffusion and annihilation, etc.) and the density of defects may therefore continue to decrease although no detailed study was performed. Numerous numerical and experimental 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 [21] and agreement with the KZ prediction in the latter [21]. See [22] 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 adiabatic regime, the typical growing length. We solely address later. Moreover, we restrict to systems with the KZ prediction.

In our endeavor to connect the dots and propose a general scenario for infinitely slow annealing. Our main conjecture, that 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 $R(t)$:

$$R(t) \simeq \xi_Q(T(t)) f \left( \frac{t}{\tau_Q(T(t))} \right).$$  

This asymptotic form encompasses equilibrium above the critical point, $x \equiv t/\tau_Q(T(t)) \ll 1$, critical coarsening, $x \propto O(1)$, and the cross-over to standard coarsening $x \gg 1$. The limits of $f(x)$ are obtained by requiring to find the expected adiabatic behavior and standard coarsening on the two extremes,

$$R(t) \simeq \begin{cases} 
\xi_Q(T(t)) & t \ll \tau_Q(T(t)) \\
[\xi_Q(T(t))]^{1 - \frac{z_d}{z}} t^{\frac{1}{z_d}} & t \gg \tau_Q(T(t)).
\end{cases}$$  

This imposes that $f(x)$ be a constant for $x \ll -1$ and proportional to $x^{1/z_d}$ for $x \gg 1$. 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 $\xi_Q$ and $R$ is shown in Fig. 1. Our scaling assumption applies to coarsening with and without
In the former case, the decaying typical number of topological defects, $N(t) \simeq R(t)^{-d}$, reads for $t \gtrsim \tau_Q$

$$N(t) \simeq \frac{\Delta g}{\tau_Q} (\xi_{eq} - \xi_{e}) - \frac{d}{\tau_Q} [1 + \nu (\xi_{eq} - \xi_{e})].$$

Note that a qualitatively similar dependence on $t$ and $\tau_Q$ was found numerically in [29] in a system with vortex-antivortex pairs. Evaluating the above expression at $t = \hat{t} = \tau_Q^{-1/\nu}$ 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, $N(t) \propto \tau_Q^{-d/\nu}$ 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 $R(\hat{t}) \simeq \rho R(-\hat{t})$ 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 during the critical coarsening from $\tau_Q^{-1}/\nu^{1/1+\nu_\xi_\xi}$ to $\tau_Q^{-2}/\nu^{1/1+\nu_\xi_\xi}$.

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 $T_r$. The typical correlation length, $R(t)$, is extracted from the analysis of the space-time correlation $C(r,t) = \langle s(\vec{x})s(\vec{x} + \vec{r}) \rangle \simeq g(r/R(t))$ 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 $R(t) = \int d^2r r^\xi C(r,t)/\int d^2r 1/r^\xi C(r,t)$ with $\zeta$ a parameter that is chosen for convenience, namely to weigh differently shorter or longer distances. In the top panel of Fig 4 we test the scaling hypothesis, eq (2), and the limits of the scaling function $f(x)$, eq. (4). 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 $|x|$. 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 4 displays $N(\tau_Q)$ and confirms the $\tau_Q^{-d/\nu}$ decay - the power is shown as a guide-to-the-eye 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 non-trivial [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 the 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 $\tau_Q$ disappears.

As a summary we analyzed the dynamic evolution induced by annealing with rate $1/\tau_Q$ ($\tau_Q \rightarrow \infty$) 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 $\tau_Q$ scaling dependence. The cross-over 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 paper 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 change drastically 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 P. Krapivsky that shows qualitative but not quantitative agreement with the KZ mechanism [30].

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