Kibble-Zurek Mechanism in the Ginzburg Regime: Numerical Experiment in the Ising Model

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Kibble-Zurek mechanism is a theory of defect formation in a non-equilibrium continuous phase transition. So far the theory has been successfully tested by numerical simulations and condensed matter experiments in a number of systems with small thermal fluctuations. This paper reports first numerical test of the mechanism in a system with large thermal fluctuations and strongly non-mean-field behavior: the two dimensional Ising model. The theory predicts correctly the initial density of defects that survive a quench from the disordered phase. However, before the system leaves the Ginzburg regime of large fluctuations most of these defects are annihilated and the final density is determined by the dynamics of the annihilation process only.

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Introduction.--- In a system with a continuous phase transition an adiabatic change of a parameter of the system, like e.g. temperature, pressure or a coupling constant in a Hamiltonian, can drive the system from a disordered phase to an ordered one. A classic example is the paramagnet-ferromagnet transition in the two dimensional (2D) Ising model. Thermodynamics of continuous phase transitions has been intensively explored over many years. Two mayor achievements: the solution of the Ising model by Onsager and the renormalization group of Wilson were rewarded with a Nobel Prize in physics. The RG formalism revealed deep connections between statistical mechanics and quantum field theory.

A candidate theory of non-equilibrium phase transitions is the Kibble-Zurek mechanism (KZM) [1,2]. Kibble pointed out [1] that in a non-equilibrium transition there is no time to fully develop the long range order characteristic for the ordered phase. As a result, the final state of the system is a mosaic of finite size ordered domains with different orientations of the order parameter in every domain. In a topologically non-trivial case this disorder takes the form of a finite density of topological defects. This qualitative idea was quantified more by Zurek [2]. Zurek mechanism is a combination of two basic facts: (1) a divergent correlation length

$$\xi \approx \xi_0 \left| \epsilon \right|^{-\nu},$$

where $\epsilon$ is a dimensionless distance from the critical point, $\nu$ is a critical exponent, and $\xi_0$ is a microscopic length scale, and (2) the critical slowing down or divergent relaxation time

$$\tau \approx \tau_0 \left| \epsilon \right|^{-\nu},$$

where $\tau_0$ is a microscopic time scale. Because of the divergent relaxation time any finite rate transition is a non-adiabatic phase transition: sufficiently close to the critical point (where $\epsilon = 0$) the system is too slow to react to the changing external parameter $\epsilon(t)$. Close to $\epsilon = 0$ we can linearize

$$\epsilon(t) = \frac{t}{\tau_Q}.$$  \hspace{1cm} (3)

The relaxation time (3) equals the transition rate $|\epsilon|/\tau_Q$ at $\epsilon_Z \approx (\tau_0/\tau_Q)^{1/\nu}$ when the correlation length (1) is

$$\xi_Z \approx \xi_0 \left( \frac{\tau_Q}{\tau_0} \right)^{1/\nu}.$$  \hspace{1cm} (4)

This Zurek length is the average size of the ordered domains after the phase transition and it determines the initial density of topological defects frozen into the ordered phase after a non-adiabatic continuous phase transition.

The original motivation for Kibble and Zurek were symmetry breaking phase transitions in cosmology. The random topological defects arising in such transitions might provide initial seeds for structure formation in the early Universe [3]. However, the universality of phase transitions makes these ideas also relevant for a wide variety of condensed matter systems where they can be verified by experiment.

The KZM prediction (4) is supported by a number of numerical simulations [4]. However, as a result of finite numerical resources these numerical data are limited to fast quenches (small $\tau_Q$) with a large $\epsilon_Z$ in the regime of small fluctuations where one can use the mean field (MF) value of the critical exponent $\nu_{MF} = \frac{1}{2}$. KZM is also supported by experiments in systems with small fluctuations like superfluid helium 3 [5], low $T_c$ superconductors [6], and fast quenches in high $T_c$ superconductors [7]. In contrast, experiments in systems with large fluctuations like helium 4 [8] or slow quenches in high $T_c$ superconductors [9] are inconclusive. Rivers suggested [10] that vortices created in the helium 4 experiment [8] disappear in a faster than expected annihilation. Due to technical difficulties the analytic calculations in Ref. [10] eventually resort to a linearization equivalent to the mean-field theory. It is suggested there that beyond this linearized theory close to the critical point the annihilation rate is divergent. However, simulations in Ref. [11] show that this effect may be not as dramatic as anticipated in Ref. [10]. These authors suggest that because of the critical
slowing down the annihilation rate close to $\epsilon = 0$ may in fact vanish. Due to limited numerical resources the numerical evidence in Ref. [11] is rather indirect. To summarize, the problem of KZM in the Ginzburg regime of large fluctuations has been recognized [10] but is far from being settled.

At the moment we do not have any condensed matter or numerical experiment supporting KZM for large fluctuations and at the same time this is the regime where KZM in principle can be questioned on general grounds. The argument leading to Eq.(4) implicitly assumes that close to the critical point the divergent correlation length $\xi$ in Eq.(1) is the only relevant length scale. However, as is well known [12] but not quite generally appreciated, if $\xi$ were the only length scale, then, on dimensional grounds, all critical exponents would take their mean field values. As they do not (for example, in the 2D Ising model $\nu = 1$ instead of the mean field $\nu_{\text{MF}} = 1/2$), then both $\xi$ and the microscopic $\xi_0$ must be relevant. With two relevant length scales the dimensional argument alone is not sufficient to determine the initial density of defects.

In this paper I report first numerical test of KZM for large fluctuations. As the critical regime is numerically demanding (large $\xi$ means large lattice and large $\tau$ means long time) I chose the simplest possible model - the celebrated 2D Ising model. This simple model has $\nu = 1$ clearly different from the mean field $\nu_{\text{MF}} = 1/2$, and it has no regime where the MF theory might be at least remotely accurate. It is a perfect testing ground for KZM.

**Ising model with Glauber dynamics.**— Hamiltonian of the ferromagnetic Ising model in 2D is

$$H = -\sum_{(i,j)} S_i S_j .$$  \hspace{1cm} (5)

Spins $S_i \in \{-1,+1\}$ sit on a 2D $N \times N$ lattice with periodic boundary conditions, $(i,j)$ means a pair of nearest neighbor sites. The microscopic lengthscale $\xi_0 = 1$ is the lattice spacing. In all the following numerical simulations a $1024 \times 1024$ lattice was used.

To study non-equilibrium phase transitions the Ising model has to be supplemented with dynamics. The standard choice is Glauber dynamics also known as Monte-Carlo with a heat bath [13]. In the Glauber algorithm every time step consists of the following sub-steps:

- choose a random spin $S_i$ from the lattice,
- calculate its local field $h_i = -\sum_{\text{n.n.}} S_j$,
- calculate a probability $P = \exp(\beta h_i)$,
- choose a random number $r \in [0,1]$,
- if $r > P$ then set $S_i = +1$, else set $S_i = -1$.

Here $\beta$ is an inverse temperature of the heat bath. This algorithm relaxes the state of the Ising model towards thermal equilibrium at a given $\beta$ [13]. On average it takes $N^2$ steps to update the state of $N^2$ spins on the lattice. These $N^2$ steps define the microscopic time scale $\tau_0$ which I set equal to 1.

The Ising model with Glauber dynamics belongs to the same universality class as the $\phi^4$ model with noise $\eta$

$$\tau_0 \frac{\partial}{\partial t} \phi = \xi_0^2 \nabla^2 \phi - \lambda(\phi^2 - 1)\phi + \eta$$  \hspace{1cm} (6)

so often employed in the numerical simulations of KZM [4]. Here the continuum real field $\phi$ is a coarse grained lattice spin $S_i$. The Ising model is an efficient “molecular dynamics” version of the $\phi^4$ field theory (6).

**Relaxation time.**— In order to estimate the exponent $y$ in Eq.(2) the relaxation time $\tau$ was measured for several values of $\beta < \beta_c$. For each $\beta$ the Ising model was initially prepared in a fully polarized state with all $S_i = 1$, and then its average magnetization $M = \sum_i S_i/N^2$ relaxed towards the equilibrium at $M = 0$, see the insert in Fig.1. Each magnetization decay was fitted with an exponent $M = \exp(-t/\tau)$. The best fits of $\tau$ are shown in the double logarithmic Fig.1 as a function of $\beta_c - \beta$. The slope of the linear fit in Fig.1 gives an estimate of $y = 2.09 \pm 0.02$.

**Quenches.**— Phase transitions were simulated with a linear ramp of the inverse temperature

$$\beta(t) = 1.5 \frac{t}{\tau_Q} .$$  \hspace{1cm} (7)

The initial state at $t = 0$ was a state with random mutually uncorrelated spins - the state of equilibrium at $\beta = 0$. Fig.2 shows density of domain walls separating positive $S_i$ from negative $S_i$ as a function of $\beta$ for a number of different transition times $\tau_Q$. The critical point is $\beta_c = 0.4407$. For large $\tau_Q$ the density plots approach
the equilibrium density \( n_{eq}(\beta) \). Note that the equilibrium density \( n_{eq}(\beta) \) of domain walls remains nonzero even for \( \beta > \beta_c \). This is the critical Ginzburg regime of large fluctuations. A non-equilibrium transition with a finite \( \tau_Q \) results in an additional non-equilibrium density \( \dot{n}(\beta) = n(\beta) - n_{eq}(\beta) > 0 \). KZM predicts that

\[
dn_{KZM}(\beta) \approx \xi_z^{-1} = \tau_Q^{-0.324 \pm 0.003}. \quad (8)
\]

Before this prediction is compared with the numerical data in Fig.2, let me digress on annihilation of domain walls.

**Defect annihilation.**— First example is annihilation of defects from an initially totally random spin configuration. The initial \( \dot{n}(t=0) \) decays in time. Fig.3 shows the equilibrating \( n(t) \) for several values of \( \beta > \beta_c \). Each decay is fitted with a solid line that follows the power law \( \dot{n}(t) = (\tau_a/\tau_0)^{1/2} \) with an exponent of 1/2 known from the theory of phase ordering kinetics [14].

The best fits are \( \tau_a = 0.86 \pm 0.05, 0.93 \pm 0.05, 0.64 \pm 0.05 \) for \( \beta = 0.47, 0.60, 1.0 \) respectively. They are more or less constant in the considered range of temperatures: as the critical point is approached the time scale for annihilation \( \tau_a \) neither diverges (as suggested in Ref. [10]) nor vanishes (as suggested in Ref. [11]), but remains finite and close to the microscopic \( \tau_0 = 1 \).

\[
\tau_a \approx \tau_0. \quad (9)
\]

The quench time \( \tau_Q \) determines the time available for defect annihilation. At late times after the transition, when most of the initial KZM domain walls are already annihilated, we expect the scaling

\[
\dot{n}(\beta) \approx \left( \frac{\tau_0}{\tau_Q} \right)^{\nu}. \quad (10)
\]

It also follows from a phenomenological equation: \( \tau_0 \frac{dn}{dt} = -\frac{1}{2}dn^3(t) \). Its solution is

\[
dn(t) = \frac{dn(0)}{\sqrt{1 + t/\tau_0}} \cdot \sqrt{dn^2(0)}.
\]

Note that at late times \( dn(t) \) is forgetting its initial value \( dn(0) = dn_{KZM} \). This solution is an illustration of the exact result (10) from Ref. [14].

Second example is annihilation of domain walls from an initial state of equilibrium at \( \beta > \beta_c \). The initial state was prepared by starting from fully polarized spins, all \( S_i = 1 \), and then heating them up at \( \beta = 0.45 \) for a time of \( 10^5 \) sufficient to reach thermal equilibrium with \( n_{eq}(0.45) \approx 0.2 \). Then at \( t = 0 \beta \) was suddenly increased (the heat bath was cooled) to \( \beta = 0.55 \). Fig.3 shows \( n(t) \) decaying towards the new equilibrium at \( n_{eq}(0.55) = 0.075 \). This decay is much faster than for random initial spins because the equilibrium domain walls in the Ginzburg regime at \( \beta > \beta_c \) are just boundaries of bubbles of the minority spin-down phase in the spin-up polarized ferromagnet. The bubbles together with their walls decay soon after the temperature is turned down.

**KZM versus annihilation.**— Figure 4 is a double logarithmic plot of the non-equilibrium density \( \dot{n}(\beta) \) in Fig.2 as a function of \( \tau_Q \) for a number of \( \beta_s \). The slope at the critical \( \beta_c = 0.4407 \) is \( -0.315 \pm 0.007 \). This slope is consistent with the KZM slope (8) of \( -0.324 \) and very different from a mean-field KZM slope of \( -0.65 \) for \( \tau_{MF} = 1/2 \). The initial non-equilibrium density of domain walls is determined by KZM.

In contrast, similar slopes for \( \beta = 1.0 \) and 1.5 are \( -0.45 \pm 0.01 \) and \( -0.48 \pm 0.01 \) respectively, and they are consistent with the phase ordering kinetics exponent of \(-1/2 \) in Eq.(10). Apparently at later times the system
forgets the initial density \(dn_{KZM}\) and \(dn(\beta)\) is determined solely by the dynamics of defect annihilation.

Indeed, the circles in Fig.4 show \(dn(\beta = 1.5)\) for a simulation where \(\beta(t)\) is ramped up like in Eq.(7), but starting from the initial \(\beta_0 = 0.6 > \beta_c\). The spins were random at the initial \(\beta_0\). The circles sit on the solid line which is a fit to \(dn(\beta = 1.5)\) obtained from a full quench like in Eq.(7). The annihilation dominated \(dn(\beta)\) at later times is not sensitive to the details of the KZM of defect formation, compare Eqs.(10,11).

However, the defects that survive annihilation at later times are KZM defects quenched in from the disordered phase. As we have already seen, compare Fig.3, that annihilation of the Ginzburg domain walls is much faster than annihilation of defects from the initially random spin state. The latter state contains large domain walls while in the former domain walls are boundaries of bubbles of a minority spin phase. The points in Fig.(4) connected by a dashed line show \(dn(\beta = 1.5)\) after a quench starting from the equilibrium state at \(\beta_0 = 0.47\) in the Ginzburg regime. These densities are orders of magnitude lower than densities from the full quenches starting at \(\beta = 0\): Ginzburg defects do not survive annihilation.

Figure 4. \(y = \log_{10} dn(\beta)\) as a function of \(x = \log_{10} \tau_0\) for \(\beta = 0.4407, 1.0, 1.5\) from top to bottom. Solid lines are the best linear fits with slopes of \(-0.315 \pm 0.007, -0.45 \pm 0.01, -0.48 \pm 0.01\) respectively. Circles show \(dn(\beta = 1.5)\) in a quench starting from \(\beta_0 = 0.6\) and random initial spins. The points connected by a dashed line show densities \(dn(\beta = 1.5)\) in a quench starting from \(\beta_0 = 0.47\) in the Ginzburg regime and spins initially in thermal equilibrium.

**Conclusion.**—I presented first numerical test of the Kibble-Zurek mechanism (KZM) in the Ginzburg regime of large thermal fluctuations. In this regime both the Zurek length \(\xi_Z\) and the microscopic length \(\xi_0\) are relevant length scales that determine the density of defects. However, the density of non-equilibrium defects frozen into the ordered phase by a quench from the disordered phase is determined by \(\xi_Z\) only. This initial density of defects is gradually annihilated and when the system leaves the Ginzburg regime the density of defects is no longer sensitive to the details of the KZM, but it is determined by the dynamics of the annihilation process only. In particular, the dependence of the density on the transition rate is determined by an exponent that comes from the theory of phase ordering kinetics and not from the KZM. The only way to see the KZM scaling (8) directly is to measure the amount of disorder close to the critical point where the non-equilibrium KZM density is largely obscured by the prevailing equilibrium thermal fluctuations. However, the defects that survive the annihilation are the KZM defects quenched in from the high temperature phase, the defects quenched in from the Ginzburg regime decay much faster. The surviving defects are a clear, though indirect, signature of the KZM.

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