KIBBLE–ŻUREK MECHANISM IN THE GINZBURG REGIME: NUMERICAL EXPERIMENT IN THE ISING MODEL

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(Received April 16, 2004)

Kibble–Żurek 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.

PACS numbers: 11.27.+d, 05.70.Fh, 98.80.Cq

1. 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–Żurek 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 Żurek [2]. Żurek mechanism is a combination of two basic facts: (1) a divergent correlation length

$$\xi \approx \xi_0 |\varepsilon|^{-\nu} , \tag{1}$$

where ε is a dimensionless distance from the critical point, ν is a critical exponent, and ξ_0 is a microscopic length scale, and (2) the critical slowing down or divergent relaxation time

$$\tau \approx \tau_0 |\varepsilon|^{-y} . \tag{2}$$

Here τ_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 $\varepsilon = 0$) the system is too slow to react to the changing external parameter $\varepsilon(t)$. Close to $\varepsilon = 0$ we can linearize

$$\varepsilon(t) = \frac{t}{\tau_{\mathrm{Q}}} . \tag{3}$$

The relaxation time (2) equals the transition rate $|\varepsilon/\frac{d\varepsilon}{dt}|$ at $\varepsilon_Z \approx (\tau_0/\tau_{\mathrm{Q}})^{\frac{1}{y+1}}$ when the correlation length (1) is

$$\xi_Z \approx \xi_0 \left(\frac{\tau_{\mathrm{Q}}}{\tau_0}\right)^{\frac{\nu}{y+1}} . \tag{4}$$

This Żurek 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 Żurek 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 τ_{Q}) with a large ε_Z in the regime of small fluctuations where one can use the mean field (MF) value of the critical exponent $\nu_{\mathrm{MF}} = \frac{1}{2}$. 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 $\varepsilon = 0$ 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 ξ in Eq. (1) is the only relevant length scale. However, as is well known [12] but not quite generally appreciated, if ξ 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 $\nu_{\rm MF} = \frac{1}{2}$), then both ξ and the microscopic ξ_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 ξ means large lattice and large τ 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 $\nu_{\rm MF} = 1/2$, and it has no regime where the MF theory might be at least remotely accurate. It is a perfect testing ground for KZM.

2. Ising model with Glauber dynamics

Hamiltonian of the ferromagnetic Ising model in 2D is

$$H = -\sum_{\langle i,j \rangle} S_i S_j \,. \tag{5}$$

Spins $S_i \in \{-1, +1\}$ sit on a 2D $N \times N$ lattice with periodic boundary conditions, $\langle i, j \rangle$ means a pair of nearest neighbor sites. The microscopic

lengthscale $\xi_0 = 1$ is the lattice spacing. In all the following numerical simulations a 1024×1024 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 $h_i = -\sum_{j \text{ n.n. } i} S_j$,
- 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 β is an inverse temperature of the heat bath. This algorithm relaxes the state of the Ising model towards thermal equilibrium at a given β [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 τ_0 which I set equal to 1.

The Ising model with Glauber dynamics belongs to the same universality class as the ϕ^4 model with noise η

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

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

3. Relaxation time

In order to estimate the exponent y in Eq. (2) the relaxation time τ was measured for several values of $\beta < \beta_c$. For each β 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 τ 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 $y = 2.09 \pm 0.02$.

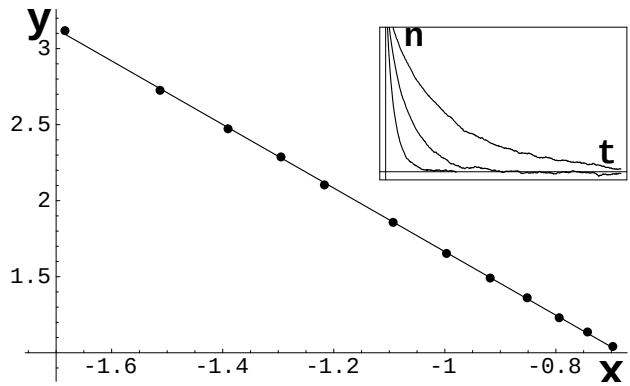

Fig. 1. $y = \log_{10}\tau$ as a function of $x = \log_{10}(\beta_c - \beta)$. The τs are the best fits to the exponential decays of magnetization shown in the insert. The solid line is the best linear fit with a slope of $y = 2.09 \pm 0.02$.

4. Quenches

Phase transitions were simulated with a linear ramp of the inverse temperature

$$\beta(t) = 1.5\frac{t}{\tau_Q}\,. \tag{7}$$

The initial state at $t = 0$ was a state with random mutually uncorrelated spins — the state of equilibrium at $\beta = 0$. Fig. 3 shows density of domain walls separating positive S_i from negative S_i as a function of β for a number of different transition times τ_Q. The critical point is $\beta_c = 0.4407$. For large τ_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 τ_Q results in an additional non-equilibrium density $dn(\beta) = n(\beta) - n_{eq}(\beta) > 0$. KZM predicts that

$$dn_{KZM}(\beta) \approx \xi_Z^{-1} = \tau_Q^{-\frac{\nu}{\nu+1}} \approx \tau_Q^{-0.324\pm0.003}\,. \tag{8}$$

Before this prediction is compared with the numerical data in Fig. 3, let me digress on annihilation of domain walls.

5. Defect annihilation

First example is annihilation of defects from an initially totally random spin configuration. The initial $dn(t = 0)$ decays in time. Fig. 2 shows the equilibrating $n(t)$ for several values of $\beta > \beta_c$. Each decay is fitted with a

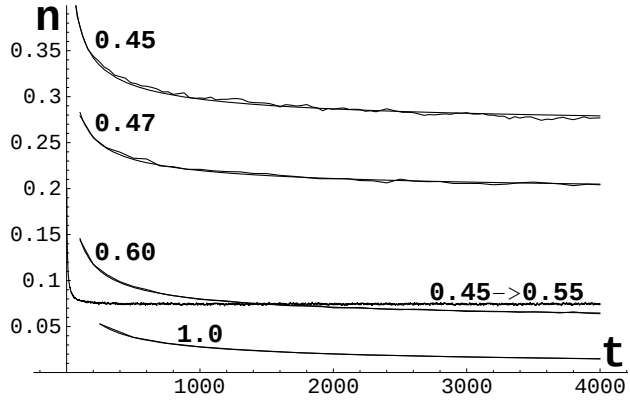

Fig. 2. Density of defects $n(t)$ starting from an initial state with random spins and decaying towards $n_{\rm eq}(\beta)$ for $\beta = 0.45, 0.47, 0.6, 1.0$. The "$0.45 \to 0.55$" marks the plot of $n(t)$ starting from the state of equilibrium at $\beta = 0.45 > \beta_{\rm c}$ in the Ginzburg regime and decaying quickly towards a new equilibrium at $\beta = 0.55$.

solid line that follows the power law $dn(t) = (\tau_a/t)^{1/2}$ with an exponent of $1/2$ known from the theory of phase ordering kinetics [14]. The best fits are $\tau_a = 1.32\pm0.20, 0.86\pm0.05, 0.93\pm0.05, 0.64\pm0.05$ for $\beta = 0.45, 0.47, 0.60, 1.0$ respectively. They are more or less constant in the considered range of temperatures: as the critical point is approached the time scale for annihilation τ_a neither diverges (as suggested in Ref. [10]) nor vanishes (as suggested in Ref. [11]), but remains finite and close to the microscopic $\tau_0 = 1$,

$$\tau_a \approx \tau_0 \,. \tag{9}$$

The quench time $\tau_{\rm Q}$ 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

$$dn(\beta) \approx \left(\frac{\tau_0}{\tau_{\rm Q}}\right)^{\frac{1}{2}} . \tag{10}$$

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

$$dn(t) = \frac{dn(0)}{\sqrt{1 + \frac{t}{\tau_0} dn^2(0)}} \,. \tag{11}$$

Note that at late times $dn(t)$ is forgetting its initial value $dn(0) = dn_{\rm KZM}$. 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 $n_{eq}(0.45) = 0.20$. Then at $t = 0$ β was suddenly increased (the heat bath was cooled) to $\beta = 0.55$. Fig. 2 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.

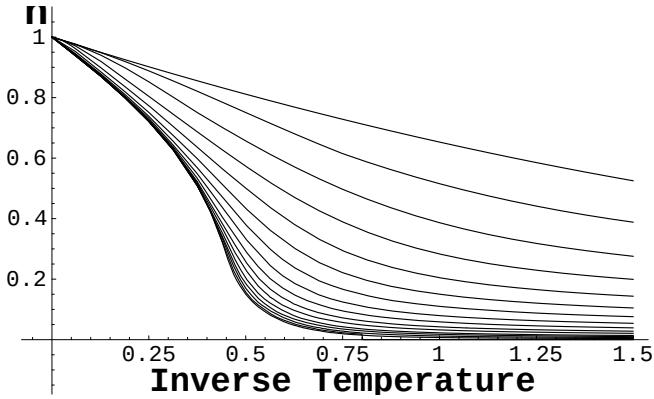

Fig. 3. Total density $n(\beta)$ of domain walls separating positive and negative S_i as a function of β for several values of the quench time $\tau_Q = 2, 4, 8, \ldots, 65536$ (from top to bottom). For the initial state of random spins the density is normalized to $n = 1$. For large τ_Q the plots tend to the equilibrium density of defects $n_{eq}(\beta)$ which is finite even for $\beta > \beta_c = 0.4407$ in the Ginzburg regime of large fluctuations.

6. KZM versus annihilation

Figure 4 is a double logarithmic plot of the non-equilibrium density $dn(\beta)$ in Fig. 3 as a function of τ_Q for a number of βs. The slope at the critical $\beta_c = 0.4407$ is -0.315 ± 0.007. This slope is consistent with the KZM slope (8) of -0.324 and different from a mean-field KZM slope of -0.25 for $\nu_{MF} = 1/2$ and $y_{MF} = 1$. 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 ± 0.01 and -0.48 ± 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 β_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. 2, 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.

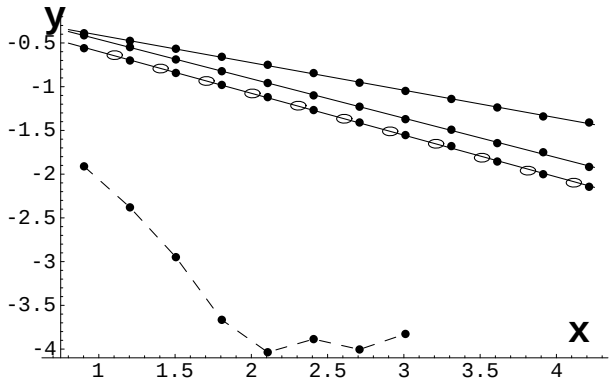

Fig. 4. $y = \log_{10} dn(\beta)$ as a function of $x = \log_{10} \tau_Q$ for $\beta = 0.4407,\ 1.0,\ 1.5$ from top to bottom. Solid lines are the best linear fits with slopes of $-0.315 \pm 0.007, -0.45 \pm 0.01, -0.48 \pm 0.01$ respectively. Circles show $dn(\beta = 1.5)$ in a quench starting from $\beta_0 = 0.6$ 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.

7. Conclusion

I presented first numerical test of the Kibble–Żurek mechanism (KZM) in the Ginzburg regime of large thermal fluctuations. In this regime both the Żurek length ξ_Z and the microscopic length ξ_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 ξ_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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