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Non-equilibrium dynamics of topological defects in the 3d O(2) model

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We present a study of the 3d O(2) non-linear σ-model on the lattice, which exhibits topological defects in the form of vortices. They tend to organize into vortex lines that bear close analogies with global cosmic strings. Therefore, this model serves as a testbed for studying the dynamics of topological defects. It undergoes a second order phase transition, hence it is appropriate for investigating the Kibble-Zurek mechanism. In this regard, we explore the persistence of topological defects when the temperature is rapidly reduced from above to below the critical temperature; this cooling (or "quenching") process takes the system out of thermal equilibrium. We probe a wide range of inverse cooling rates $\tau_{\rm Q}$ and final temperatures, employing distinct Monte Carlo algorithms. The results consistently show that the density of persisting topological defects follows a power-law in $\tau_{\rm Q}$, in agreement with Zurek's conjecture. On the other hand, at this point, our results do not confirm Zurek's prediction for the exponent in this power-law, but its final test is still under investigation.

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PoS(LATTICE2023)346

1. Kibble mechanism in the Early Universe

According to established cosmology, the period $\lesssim 10^{-12}$ s after the Big Bang — with a temperature $\gtrsim 160$ GeV — was dominated by electroweak interactions. This period ended when the Higgs field acquired its vacuum expectation value $|\langle\Phi\rangle| > 0$. The seeds of possible topological defects — in particular cosmic strings — could date back to that instant.

For their formation, Kibble suggested the following mechanism [1]: causality did not allow the complex phases of $\langle\Phi\rangle$ to be correlated in well separated regions of the Universe. Cosmic strings may have formed at the interfaces between such regions, when the phase change — integrated over a closed loop — amounted to a non-zero multiple of 2π.

The Kibble mechanism could have led to a string network of topological defects. Later, the cosmic strings could have lost some energy by gravitational radiation and particle emission, observational bounds are discussed in Ref. [2]. Still, their topological nature might have stabilized them to this day.

The attempts to observe cosmic strings have not been successful so far. They seem to be ruled out as seeds for the galaxy formation: that is incompatible with observations by the COBE and WMAP satellites of the dominant scale of anisotropies in the Cosmic Microwave Background [3]. This does, however, not imply that cosmic strings do not exist. Recently, the search for a corresponding signal focuses on gravitational waves, see *e.g.* Ref. [4].

2. Vortex lines in the 3d O(2) model

We consider the O(2) non-linear σ-model on 3-dimensional, cubic lattices of volumes $V = L^3$. At each lattice site x, there is a classical spin $\vec{e}_x = (\cos\varphi_x, \sin\varphi_x) \in S^1$ and the Hamilton function $\mathcal{H}$ has the standard form (in lattice units)

$$\mathcal{H}[\vec{e}\,] = -J \sum_{\langle xy \rangle} \vec{e}_x \cdot \vec{e}_y \,, \quad Z = \int D\vec{e}\, \exp(-\mathcal{H}[\vec{e}\,]/T)\,, \tag{1}$$

with a global O(2) symmetry. The sum runs over the nearest neighbor lattice sites, Z is the partition function and T the temperature (in units where $k_{\rm B} = 1$, and $J = 1$). We always assume periodic boundary conditions. This model undergoes a second order phase transition at $T_{\rm c} = 2.2018441(5)$ [5]. Its universality class is expected to coincide with the superfluid transition of ^{4}He, the so-called λ-transition, although there is some tension with the value of the critical exponent α [6].

For a given configuration, we assign to each plaquette, say in the $\mu\nu$ plane, the vorticity

$$v_{x,\mu\nu} = (\Delta\varphi_{x,x+\hat{\mu}} + \Delta\varphi_{x+\hat{\mu},x+\hat{\mu}+\hat{\nu}} + \Delta\varphi_{x+\hat{\mu}+\hat{\nu},x+\hat{\nu}} + \Delta\varphi_{x+\hat{\nu},x})/2\pi = \begin{cases} 1 & \text{vortex} \\ 0 & \text{neutral} \\ -1 & \text{anti-vortex} \end{cases} \tag{2}$$

where $\hat{\mu}$, $\hat{\nu}$ are the lattice unit vectors in μ- and ν-direction, and $\Delta\varphi_{xy} = \varphi_y - \varphi_x \bmod 2\pi \in (-\pi, \pi]$ (note the unusual modulo operation). Ignoring configurations with probability measure zero, each plaquette carries either a vortex, or an anti-vortex or it is neutral, as indicated in eq. (2).

The vortices form *vortex lines*, which connect centers of the lattice unit cubes. For a vortex and an anti-vortex, the connection of adjacent cubes has opposite orientation. If the continuation from a cube center is ambiguous, we make a random choice. In this manner, we obtain vortex lines, which are closed in practically all cases (taking into account the periodic boundaries), in remarkable analogy to global cosmic strings.

Figure 1 shows the mean string length and the density of the total string length, as functions of the temperature T, in thermal equilibrium. Both quantities converge well in a volume $V = L^3$, when the lattice size attains $L \approx 100$. A scale for relating them to the cosmic strings would be set by the correlation length, which corresponds to $1/m_{\rm Higgs}$. For a comprehensive study of vortex line properties as a possible order parameter (which was, however, not exactly confirmed), we refer to Ref. [7].

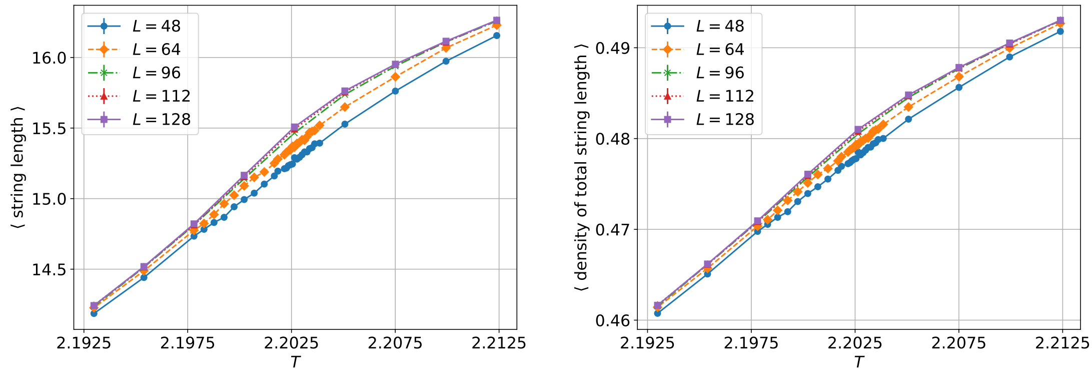

Figure 1: Properties of vortex lines in the XY model, in L^3 lattices, in analogy to cosmic strings: mean string length (left) and the fractional volume covered by strings (right), both with modest finite-size effects.

3. Kibble-Zurek mechanism in condensed matter

Zurek suggested to materialize the Kibble mechanism in condensed matter systems [8], where it is denoted as the Kibble-Zurek mechanism. Such experiments were successfully carried out in a non-linear optical system [9] and with liquid ^{4}He [10] .

The Kibble-Zurek mechanism was formulated for systems with a second order phase transition. At the critical temperature T_c, the correlation length ξ and the equilibrium relaxation time τ diverge as

$$\xi(\epsilon) = \frac{C_\xi}{|\epsilon|^\nu} \,, \quad \tau(\epsilon) = \frac{C_\tau}{|\epsilon|^{z\nu}} \,, \quad \text{where} \quad \epsilon = \frac{T - T_c}{T_c} \tag{3}$$

is the reduced temperature, C_ξ and C_τ are constants, ν is a critical exponent (in the usual notation) and z is the dynamical critical exponent.

In agreement with the literature, we consider a temperature, which linearly decreases in time t. We denote the inverse cooling (or "quenching") rate as $\tau_Q > 0$, and formulate the temperature as

$$T(t) = T_c\left(1 - \frac{t}{\tau_Q}\right) \;\rightarrow\; \epsilon(t) = -\frac{t}{\tau_Q} \;; \qquad t \in [t_i, t_f], \quad t_i = -\tau_Q \,, \quad 0 < t_f \leq \tau_Q \,, \tag{4}$$

hence the temperature decreases from its initial value $T_i = T(t_i) = 2T_c$ to $T(0) = T_c$ and finally down to $T_f = T(t_f) < T_c$.

- At an early stage, when we are still far from criticality, T is clearly larger than T_c, so the relaxation time τ is short, and for $\tau_Q \gg \tau$ the cooling is quasi-adiabatic.

- As we approach criticality, $T \approx T_c$, however, τ becomes long and the dynamics departs from equilibrium; then the system is "frozen".

Del Campo and Zurek define the transition between the quasi-adiabatic and quasi-frozen regimes at the time $\pm\hat{t}$, where the elapsed time before and after crossing criticality coincides with the relaxation time [8],

$$\tau(\hat{t}) = \hat{t} \qquad \Rightarrow \qquad \hat{t} = (C_\tau \tau_Q^{z\nu})^{1/(1+z\nu)} \ . \tag{5}$$

At time $\hat{t}$, the reduced temperature and the correlation length are given by

$$\epsilon(\hat{t}) = -\Big(\frac{C_\tau}{\tau_{\rm Q}}\Big)^{1/(1+z\nu)} \quad , \qquad \xi(\hat{t}) = C_\xi \left(\frac{\tau_{\rm Q}}{C_\tau}\right)^{\nu/(1+z\nu)} \ . \tag{6}$$

Del Campo and Zurek further estimate the density of topological defects, which persists at time $\hat{t}$ (after crossing the critical point) as

$$\rho = \xi^{\delta-d} = C_\xi^{\delta-d}\Big(\frac{C_\tau}{\tau_{\rm Q}}\Big)^{\zeta} \propto \tau_{\rm Q}^{-\zeta} \ , \qquad \zeta = \frac{(d-\delta)\nu}{1+z\nu} \ , \tag{7}$$

where d is the spatial dimension and δ is the dimension of the topological defects. Hence this assumption leads to a power-law with the exponent that we denote as ζ, $\rho \propto 1/\tau_Q^{\zeta}$.

According to Refs. [10, 11], experiments with hexagonal manganites ($R\mathrm{MnO}_3$) are in agreement with this prediction for large values of $\tau_{\rm Q}$, with $d = 3$, $\delta = 1$ and $z = 2$.

For the 3d O(2) model, we also have $d = 3$ and $\delta = 1$, but $\nu = 0.6717(1)$ [6]. If the model is simulated with a local-update algorithm, like Metropolis or heatbath, the dynamical critical exponent — with respect to the evolution in Markov time — is again known to be $z \approx 2$. Then Zurek's prediction implies

$$\zeta_{\rm Z} \approx 0.57 \ . \tag{8}$$

4. Vortex density after rapid cooling

For our numerical investigation, we first thermalize the model at a high temperature of $T = 2T_c$; this is preferably done with the cluster algorithm.

Then we switch to a local update algorithm, Metropolis or heatbath, and perform lexicographic sweeps of L^3 spin updates (here it makes indeed a difference if the updated spins are randomly selected). In the Metropolis algorithm, the entire circle S^1 is considered for a new spin direction (introducing a limited interval would mean another artificial ingredient). For the implementation of the heatbath algorithm, we follow the prescription of Ref. [12]. In this cooling process, the highly efficient cluster algorithm (which is optimal in equilibrium simulations) does not seem appropriate, because its evolution in Markov time is too quick for the cooling process to be well monitored.

After each sweep, the temperature is linearly decreased according to eq. (4), until it arrives at $T_{\rm f}$. We measure the vortex density ρ after each sweep, and repeat this cooling process 1000 times, starting every time from a different configuration, which is thermalized at $2T_c$. For each instant in Markov time, *i.e.* after each number of sweeps, we average over the values of ρ measured in these 1000 processes. We are particularly interested in the final vortex density $\rho_{\rm f}$; for rapid cooling, it is well above the equilibrium density at $T_{\rm f}$ (which vanishes for $T_{\rm f} = 0$).

A similar study was performed before in the 2d XY model [13], where, however, the phase transition is essential (infinite order in Ehrenfest's scheme), *i.e.* not of second order as Zurek assumed when formulating his conjecture.

Figure 2 shows the vortex density ρ, *i.e.* the fraction of all plaquettes that carry either a vortex or an anti-vortex, on a 96^3 lattice, during a cooling process which is linear in the Markov time t (in units of sweeps), from $T_{\rm i} = 2T_{\rm c} \simeq 4.4$ down to $T_{\rm f} = 0$, according to eq. (4). Of course, under rapid cooling — with a short inverse cooling rate $\tau_{\rm Q}$ — more vortices remain. Since the heatbath algorithm is more efficient than Metropolis, less vortices persist after the same number of sweeps.

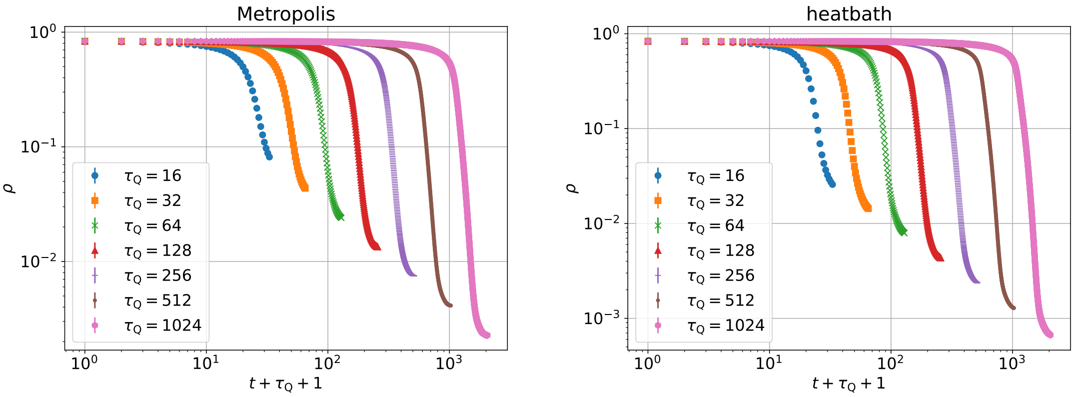

Figure 2: The vortex density ρ in a 96^3 lattice under linear cooling, from $T_{\rm i} = 2T_{\rm c}$ to $T_{\rm f} = 0$. The plots on the left and on the right refer to the Metropolis and to the heatbath algorithm, respectively. The Markov time t is given in units of lexicographic sweeps.

In Figure 3, we first show the final vortex densities $\rho_{\rm f}$, at the end of the cooling process, as a function of $\tau_{\rm Q}$, for $T_{\rm f} = 0$ and for $T_{\rm f} = 2.0642$ (just below $T_{\rm c} \simeq 2.20$). The plots above confirm the expected power-laws $\rho_{\rm f} \propto \tau_{\rm Q}^{-\zeta}$, cf. eq. (7), which is observed for all $T_{\rm f} < T_{\rm c}$, and for both algorithms.

The central plots illustrate the extrapolations of the exponent ζ, defined in eq. (7), to the thermodynamic limit $L \longrightarrow \infty$ (still referring to lattice volumes L^3). The lower plots show how the values of ζ depend on $T_{\rm f}$, at fixed L and large-L extrapolated. Zurek's prediction (8) is attained for specific final temperatures $T_{\rm f}$, but at this point this seems accidental. Careful measurements of the auto-correlation time — to be identified with the relaxation time τ — will be required to check whether or not these values are related to the cooling time $\hat{t}$ that Zurek refers to.

5. Summary and outlook

We presented simulation results for the 3d O(2) model as an effective theory for the origin of (possible) cosmic strings [1]. The vortices form closed loops, like global cosmic strings. We measured their mean length and density in thermal equilibrium, as functions of temperature.

We monitored the vortex density ρ under rapid cooling, across the critical temperature $T_{\rm c}$, which takes the system out of equilibrium. Both with the Metropolis and with the heatbath algorithm, the finally persisting density $\rho_{\rm f}$ follows a power-law in the cooling rate, as predicted by Zurek [8]. The characteristic exponent ζ depends somewhat on the algorithm and on the final temperature $T_{\rm f} < T_{\rm c}$.

A detailed study of the specific value of $T_{\rm f}$, at which Zurek predicts the value of $\zeta_{\rm Z}$ in eq. (8), remains to be performed. The verification of his value depends on exhaustive measurements of the auto-correlation time, which takes the role of the relaxation time τ.

PoS(LATTICE2023)346

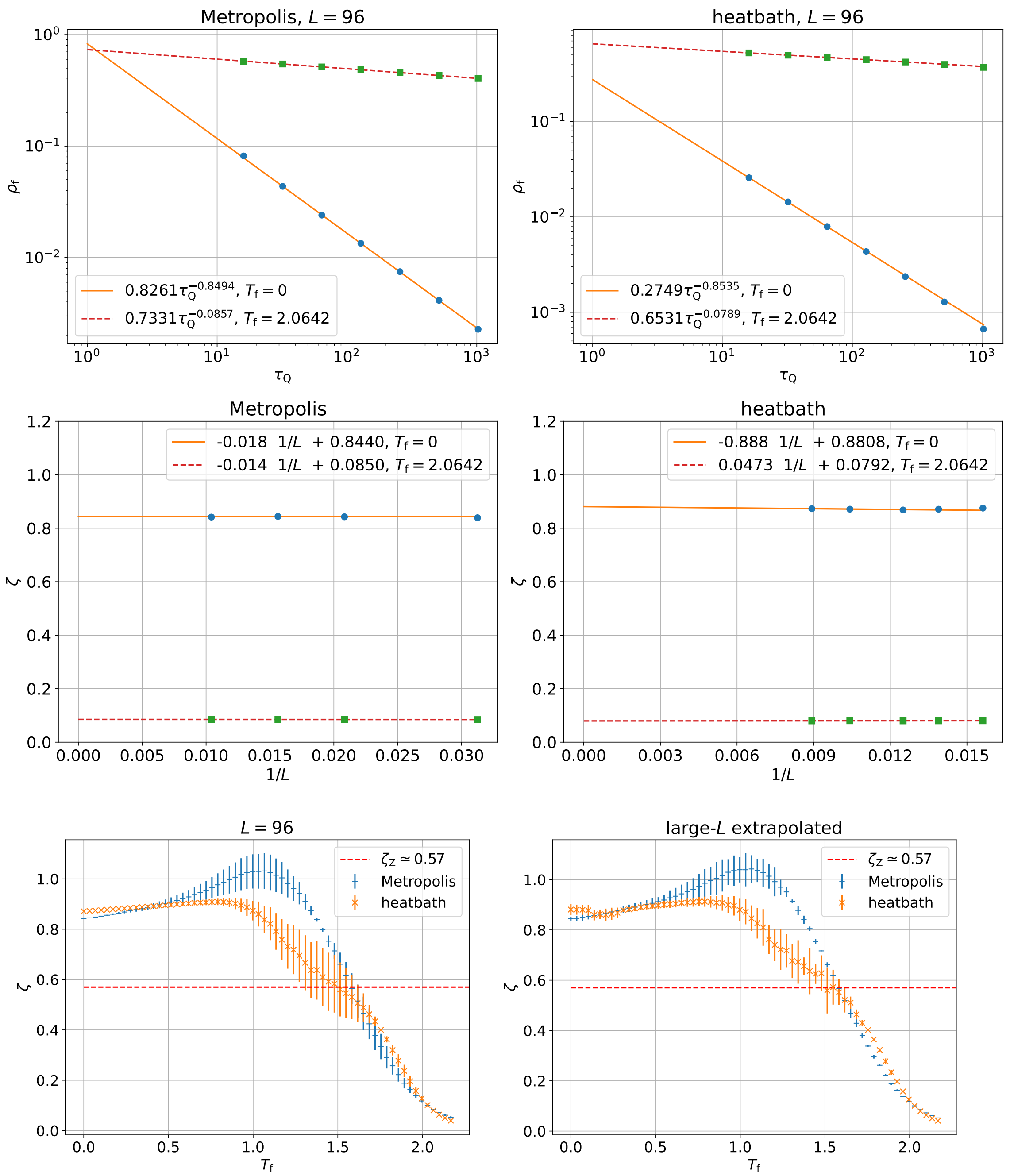

Figure 3: Above: The persisting vortex density ρ_f at the end of a rapid cooling process down to two values of $T_f < T_c$, in a lattice volume 96^3. In each case, ρ_f follows a power-law in τ_Q, in agreement with eq. (7), $\rho_f \propto \tau_Q^{-\zeta}$. Center: Large-$L$ extrapolations of the corresponding exponent ζ. Bottom: Dependence of the ζ-value on T_f, in a fixed lattice volume of 96^3 (left) and large-L extrapolated (right), compared to Zurek's prediction ζ_Z in eq. (8).

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