Topological defects in the O(2) model out of equilibrium

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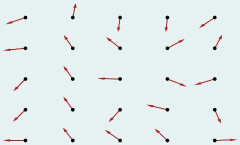
Introduction

- The classical O(2), or XY, lattice model is defined by the Hamiltonian



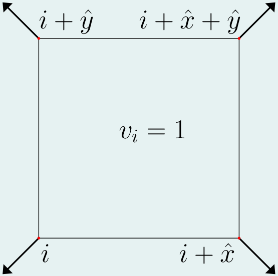
$$H = -J \sum_{\langle ij \rangle} \vec{\sigma}_i \cdot \vec{\sigma}_j = -J \sum_{\langle ij \rangle} \cos(\theta_i - \theta_j), \quad \vec{\sigma}_i \in \mathbb{S}^1, \quad V = L^D.$$

- The 2D model undergoes a *topological phase transition* driven by the topological defects of the system (vortices). The vorticity of a plaquette is defined as

$$v_i = \frac{1}{2\pi} \left(\Delta\theta_{i,i+\hat{x}} + \Delta\theta_{i+\hat{x},i+\hat{x}+\hat{y}} + \Delta\theta_{i+\hat{x}+\hat{y},i+\hat{y}} + \Delta\theta_{i+\hat{y},i} \right),$$

$$\Delta\theta_{i,j} \equiv (\theta_j - \theta_i) \bmod 2\pi \in (-\pi, \pi],$$

$$v_i \in \{-1, 0, 1\}.$$



$v_i = 1$ represents a vortex and $v_i = -1$ represents an anti-vortex.

- The 3D model undergoes a second order phase transition

$$\xi = \frac{C_\xi}{|\epsilon|^\nu} \quad \rightarrow \quad \text{correlation length},$$

$$\tau = \frac{C_\tau}{|\epsilon|^{z\nu}} \quad \rightarrow \quad \text{relaxation time},$$

where C_ξ and C_τ are constants, $\epsilon \equiv (T_c - T)/T_c$, ν is a *critical exponent* and z is known as the *dynamical critical exponent*. The latter depends on the dynamics of the system.

- We study the dynamics of the vortex density after a linear cooling process at different speeds by means of Monte Carlo simulations.

Zurek's mechanism

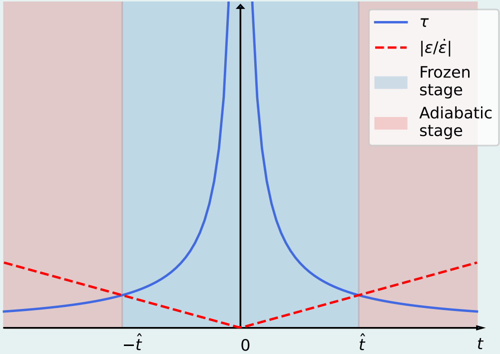
- Consider a system that undergoes a second order phase transition and linearly cool it with time according to

$$\epsilon(t) = \frac{t}{\tau_Q} \quad \text{or} \quad T(t) = T_c\left(1 - \frac{t}{\tau_Q}\right), \quad t \in [-\tau_Q, \tau_Q],$$

where τ_Q is known as the *inverse cooling rate*.
$T(-\tau_Q) = 2T_c, \quad T(0) = T_c, \quad T(\tau_Q) = 0.$

- Zurek gives a prediction for the density of topological defects at the transition between the adiabatic and frozen stages, *i.e.* at $\hat{t}$ [1,2]

$$\rho \propto \left(\frac{1}{\tau_Q}\right)^{\frac{(D-d)\nu}{1+z\nu}} \equiv \left(\frac{1}{\tau_Q}\right)^{-\zeta}.$$



[1] W. H. Zurek. *Nature*, **317**:505–508, (1985).

[2] A. del Campo and W. H. Zurek. *Int. J. Mod. Phys. A*, **29**:1430018, (2014).

Remarks

- Zurek's prediction is valid only for second order phase transitions, where the correlation length and the relaxation time have a power-law behavior in $\epsilon = (T_c - T)/T_c$ in the vicinity of T_c.

- In practice, the determination of $\hat{t}$ is ambiguous.

- Several experiments have attempted to verify Zurek's prediction for the density of topological defects. Some of them successfully verified the power-law dependence on the inverse cooling rate [3,4,5]. To deal with the ambiguity of $\hat{t}$, most works measure the density of topological defects at a final temperature after cooling the system under the critical temperature.

[3] S. Ducci *et al.* *Phys. Rev. Lett.*, **83**:5210– 5213, (1999).

[4] S. Casado *et al.* *Phys. Rev. E*, **63**:057301, (2001).

[5] S.-Z. Lin *et al.* *Nat. Phys.*, **10**:970-977, (2014).

Markov chains and Monte Carlo simulations

- One is usually interested in computing expectation values

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \mathrm{Tr}\left(\mathcal{O} e^{-\beta \hat{H}} \right), \quad \beta = \frac{1}{T}, \quad Z = \mathrm{Tr}\left(e^{-\beta \hat{H}} \right).$$

- Monte Carlo methods generate configurations $[\sigma]$ distributed according to

$$p[\sigma] = \frac{1}{Z} e^{-\beta H[\sigma]}.$$

  This way, one can determine $\langle \mathcal{O} \rangle$ through

$$\langle \mathcal{O} \rangle \approx \frac{1}{N} \sum_{[\sigma]} \mathcal{O}[\sigma],$$

  where N is the number of configurations sampled with probability $p[\sigma]$.

- Monte Carlo simulations rely on *Markov chains*, which are sequences of configurations where the $t+1$ configuration only needs the information of the t configuration to be created

$$[\sigma_1] \to [\sigma_2] \to \cdots \to [\sigma_t] \to [\sigma_{t+1}] \to \cdots$$

  To achieve this one requires a transition probability independent of t

$$T(\sigma' = \sigma_{t+1}|\sigma_t) = T(\sigma'|\sigma), \quad \text{(probability of moving from } [\sigma] \text{ to } [\sigma'])$$

$$\sum_{[\sigma']} T(\sigma'|\sigma) = 1.$$

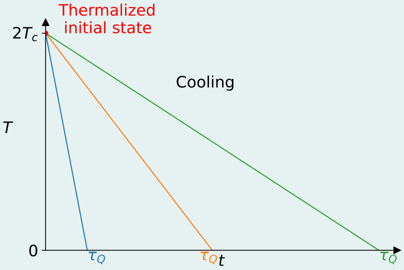
- For the configurations to reach the equilibrium probability, $p[\sigma]$, the following equation must be fulfilled

$$p[\sigma] = \sum_{[\sigma']} p[\sigma']T(\sigma|\sigma').$$

  A condition to satisfy this is *detailed balance*

$$T(\sigma'|\sigma)p[\sigma] = T(\sigma|\sigma')p[\sigma'].$$

Simulation out of equilibrium



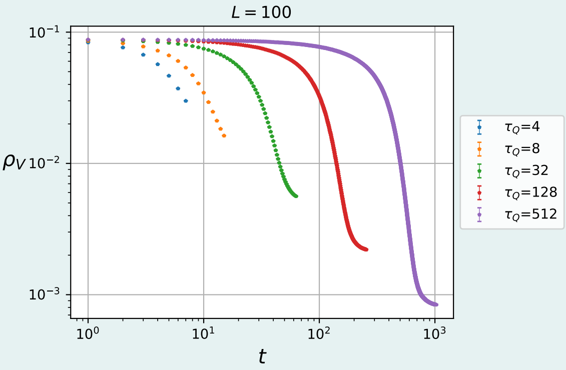
- Thermalize the system at $2T_c$.
- Update the system with a Monte Carlo algorithm, but for each new configuration lower the temperature according to

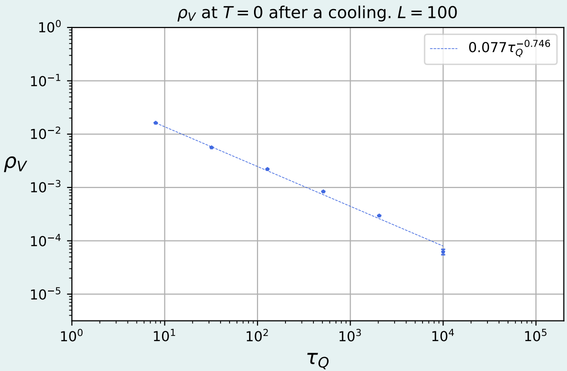
$$T(t) = T_c \left(1 - \frac{t - \tau_Q}{\tau_Q}\right), \quad t \in [0, 2\tau_Q].$$

  We measure the evolution of an observable with the temperature.
- Repeat the two previous steps numerous times to generate a good statistics of the evolution of an observable during the cooling.

We are particularly interested in the dynamics of the density of vortices, ρ_V.

Cooling in two dimensions with the Metropolis algorithm

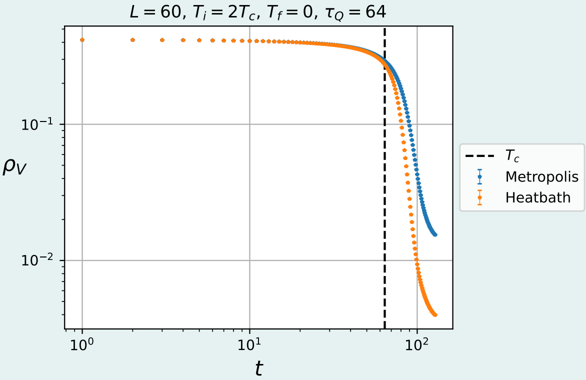


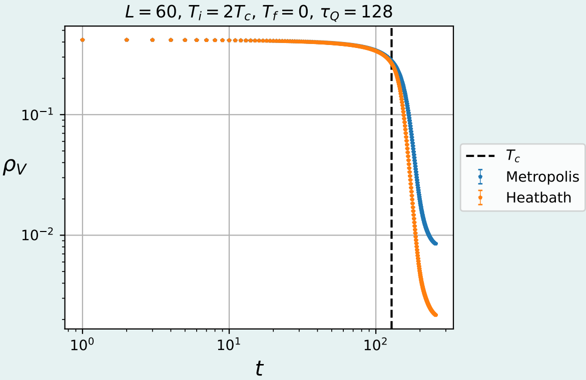


- Zurek's prediction does not apply for the 2D XY model.
- Ref. [6] claims that $\rho_V(T = 0)$ follows a logarithmic decay in τ_Q instead of a power-law. Still, for $\tau_Q \gg 1$ it can be effectively considered as a power-law. They found $\rho_V(T = 0) \propto \tau_Q^{-0.72}$.

[6] A. Jelić and L. F. Cugliandolo. *J. Stat. Mech. Theory Exp.*, **2011**:P02032, (2011).

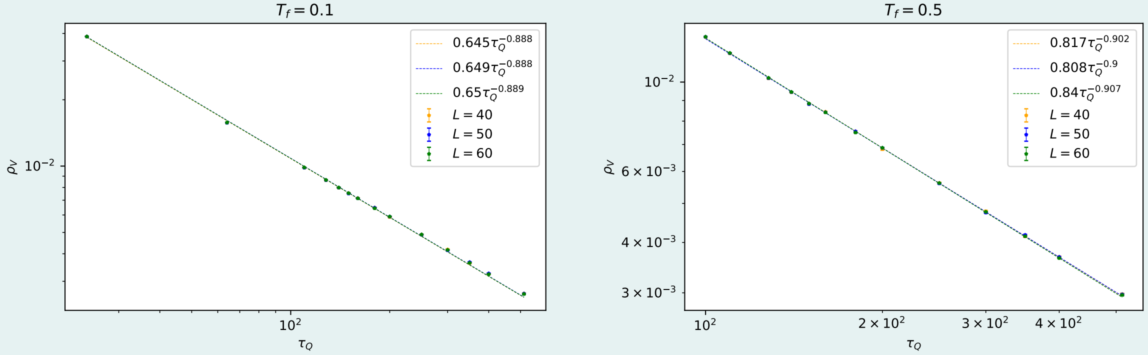
Cooling in three dimensions





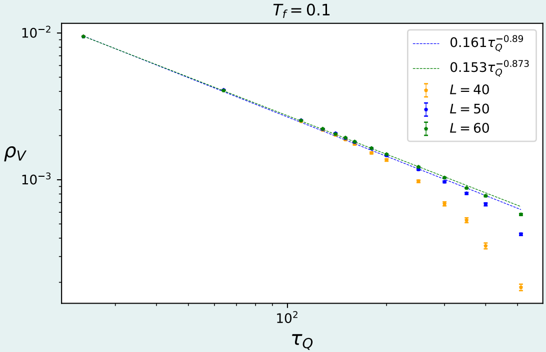
Power-law decay

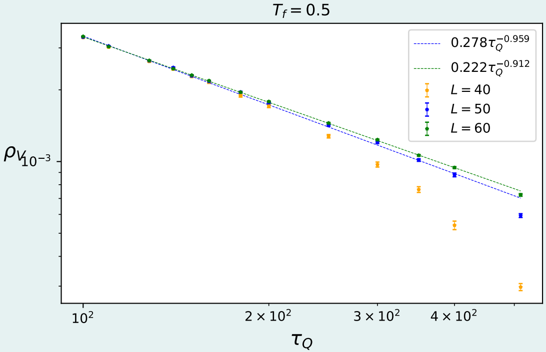
Metropolis algorithm



$$T_c \simeq 2.2018$$

Heatbath algorithm





$$T_c \simeq 2.2018$$

- For the 3D XY model $\nu = 0.67169(7)$[7] and for the heatbath and Metropolis algorithms $z \approx 2$ [8]. Then, Zurek's prediction is $\rho_V \propto \tau_Q^{-(D-d)\nu/(1+z\nu)} = \tau_Q^{-\zeta} = \tau_Q^{-0.5733}$ after cooling below the critical temperature. We obtain the following exponents

T_f	Metropolis	Heatbath
0.001	0.8705(57)	1.0313(336)
0.01	0.8531(23)	0.9277(117)
0.1	0.8889(34)	0.8734(42)
0.2	0.8952(47)	0.8829(38)
0.3	0.8905(30)	0.8984(58)
0.4	0.8911(22)	0.9103(56)
0.5	0.9073(35)	0.9116(49)
0.6	0.9181(34)	0.9077(43)

[7] M. Campostrini, M. Hasenbusch, A. Pelissetto and E. Vicari. *Phys. Rev. B*, **74**:144506, (2006).

[8] M. Hasenbusch. *Phys. Rev. E*, **101**:022126, (2020).

Conclusions

- The results show that the density of vortices follows a power-law decay in τ_Q when we cool the system down to temperatures $T \ll T_c$, as predicted by Zurek. However, we do not obtain the scaling exponent, ζ, that he predicts.
- The power-law is a generic property for cooling out of equilibrium, independently of the algorithm. This is consistent with experiments too.
- The ideas here presented could be applied to other early universe models to estimate the density of cosmic strings in the cosmos.
- A comparison between simulations and experiments out of equilibrium is not straightforward, because we do not know exactly how the dynamics of nature out of equilibrium works. Still, one would expect the exponent ζ to be universal.