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Kibble-Zurek Scaling with Matrix Product States

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Abstract. We study the dynamics of second-order phase transitions that may have taken place in the early universe and analyze the Kibble-Zurek (KZ) scaling as well as the formation of topological defects emerging from a quench in the one-dimensional Bose-Hubbard model. We describe the universal dynamics of the KZ mechanism (KZM) and the topological defect formation by simulating the Bose-Hubbard model at zero temperature. We study the effects of thermalization on the ground state by analyzing the transition between Mott and superfluid phases. The out-of-equilibrium dynamics induced by a quench of the hopping parameter is presented. We find a KZ scaling behaviour at zero temperature and analyze the KZ dynamics.

1. Introduction

In the early Universe after the Big Bang, cosmological phase transitions may have been generated by the expansion and cooling of the Universe. During this transitions, the symmetry of vacuum was broken and new vacuums within spacelike separated regions were formed. A challenging problem in current cosmology is whether the vacuum contains these topological defects forming during phase transitions in the early universe and occurring within 10–35s after the Big Bang in grand unified theories. After the cosmological phase transition at 10²⁷K, the a phase of the vacuum is disordered, possibly giving rise to a number of topological defects. The cosmological mechanism behind these processes can be observed in condensed matter systems under certain conditions in laboratory. In condensed matter theory, when a physical system is rapidly driven through a second-order phase transition, topological defects (vortices, strings) are created at a density that is dependent on the speed of the underlying transition.

The KZ theory [1] predicts a variety of transformations from high- to low-temperature phases, associated with a spontaneous symmetry breaking and the evolution of topological defect structures like domain walls, strings, and monopoles. Cosmic strings may be directly related to the primordial density inhomogeneities that later gave rise to galaxy formation. These processes are also important for their connection to the grand unified theory (GUT) symmetry-breaking phase transition of the very early universe. GUT phase transition may have played a significant role in the inflationary dynamics of the early Universe. T. W. B. Kibble suggested [2] that such defect structures (domain walls, strings, and monopoles) may have appeared during the expansion and cooling of the early and very early universe. In recent years, most current experiments based on ion-crystals, spin-liquids, liquid ³He, liquid ⁴He, superconducting films, polariton superfluids, Josephson tunnel junctions and ultra cold atoms in optical lattices contain numerous findings with different levels of certainty which are consistent with existing quantitative KZM predictions [3]. KZM model [4] model has been applied to different scales from cosmological concepts to atomic systems, such as the Higgs field in the very early universe, superconductors or quantum fluids in condensed matter systems. The predicted behaviour at cosmological scale is present in laboratory when a system going through a second-order



phase transition is cooled at a finite rate into the low symmetry phase. Cosmological inflationary theories have grown popularity mainly due to the lack of such defects within the visible cosmological horizon. We simulate the Kibble–Zurek mechanism [5] using Matrix product states simulations of the Bose–Hubbard model and discuss its nonequilibrium dynamics behaviour on the background of a cosmological evolution scenario. Within this picture, we investigate the nonequilibrium dynamics in a condensed matter analog of the inflationary dynamics of the Early Universe. The Kibble–Zurek mechanism [6] provides a description of the topological defect structure occurring during the symmetry breaking phase transitions, resulting in the presence of cosmological strings in the early universe or vortex lines in a superfluid. Specifically, ultracold atoms in optical lattices provide a unique setup to study the non-equilibrium quantum dynamics of defect structure formation. The recent progress in ultracold atoms physics provides key experiments for non-equilibrium dynamics and quantitative testable solutions for isolated, versatile and highly controllable systems. For example, a quench in pressure at a finite rate will drive liquid ^4He from a normal phase to a superfluid phase, leaving behind vortex lines, that may be associated with the existence of cosmic strings in the Early Universe. The defect structure is generated by the cooling processes when spatially separated domains are placed too far apart to exchange any information, due to finite communication speed allowed, resulting in multiple separated space-time regions with degenerated local broken symmetry [7]. The prediction of the formation of defects across a quantum critical point provides an intuitive theoretical framework for quasi-adiabatic quench processes across quantum phase transitions [8]. Kibble–Zurek hypothesis [9] provides a method to calculate the density of such defects when their symmetries are present, allowing to find the scaling laws for the density of defects as a function of the quenching rate through the phase transition and predict the growth of correlations and the density of defects following an asymptotically slow ramp.

We analyze the defect and domain structure quantitatively via Matrix Product States for Bose–Hubbard model [10] in a lattice regularised model. The mechanism describes the the nonequilibrium dynamics associated with the symmetries and the scaling laws after a phase transition, as long as its effects dominate the kinetics of the topological defect formation. The resulting dependence of the size of the causal domains where symmetry is overall broken is given by a power law with a small fractional exponent. The main prediction of this mechanism is the scaling of the defect density with the quench rate. During recent years, several experiments and numerical simulations studying the formation of defects in phase transitions induced by a quench both were carried out. Most systems of bosons in an optical lattice are well described by the Bose–Hubbard model, used in studying the superfluid to Mott insulator phase transition and realized in a multitude of experiments. The one-dimensional Bose–Hubbard model is particularly interesting because of the presence of a multicritical point with a Berezinskii–Kosterlitz–Thouless (BKT) transition. Findings from numerical simulations of the KZM scaling law [11] for exponents of the correlation length and the rate of topological defect formation with respect to the quench time are of direct relevance to the study of non-equilibrium behavior in cosmological scenarios. At the same time, the confirming experiments with ultra-cold atomic gases represent a step forward towards a better understanding of the broken symmetry vacuum, spontaneous formation of topological defects and the associated dynamical phase transitions in the early universe.

2. Topological defect formation and the Kibble-Zurek mechanism

The formation of topological defects predicted by field theory in cosmology lead to important consequences for the evolution of the Early Universe, associated to relativistic causality. KZM mechanism was mainly developed to predict the power-law scaling of the defect density across a continuous quantum phase transition. The adiabatic-impulse approximation tool approximates the time evolution of the quantum state of the system and has its origin in KZM theory applied to continuous quantum phase transitions. Spontaneous symmetry breaking assumes the degeneracy of the ground state of the system. When the system goes out of equilibrium, the broken symmetry phase contains different spatial regions defined by the different orientations of the broken symmetry. Therefore, in the new phase, independent choices of the vacuum will be associated with causally disconnected regions in the extended system. KZM scenario [12] is associated with nonequilibrium dynamics and second

order phase transitions, as well as estimating the density of defects as a function of the quench rate through this transition. In quantum field theory, phase transitions are defined as transitions between one vacuum state and another. A quantum phase transition is a transition that is driven by quantum mechanical and not by thermal fluctuations. As a system approaches the absolute zero temperature, the thermal fluctuations are frozen out, and the quantum mechanical behaviour becomes relevant. If the Universe is in absolute ground state at a finite temperature, as it slowly cools, the ground state evolves continuously through what is known as a second order phase transition (or a continuous phase transition). If this change in the ground state of the quantum field is sudden and discontinuous, a first order phase transition occurs. When the change in temperature is slow compared with the relaxation time, the order parameter has to time to adjust to this change, and the evolution will be adiabatic. KZM predicts that the density of the topological defects in a second order phase transition should scale with the transition rate. The defects are mainly developing because of the divergence of the relaxation time near a critical point, resulting in a nonequilibrium dynamical process when the system is not able to follow the changes, causing the symmetry to be broken. During a non-equilibrium continuous phase transition, the evolution ceases to be adiabatic near a critical point as a result of a slowing down dynamics associated with the divergence of the relaxation time close to the critical point. When the system is smoothly driven from a disordered to an ordered phase through a second order phase transition, topological defects are formed and the scaling exponent of the defect density with the quench rate can be predicted by KZM.

We study the defect production upon slowly changing a system parameter. Let us assume that when crossing of the phase transition at a finite rate, the spontaneous symmetry breaking during a continuous second-order phase transition is controlled by a parameter λ . KZM will describe the dynamical evolution of a continuous phase transition under a time-dependent change of λ across the critical value. The evolution is characterized by the divergence of the correlation length ξ at equilibrium

$$\xi(\varepsilon) = \frac{\xi_0}{|\varepsilon|^\nu}, \quad (1)$$

as well as the relaxation time at equilibrium τ

$$\tau(\varepsilon) = \frac{\tau_0}{|\varepsilon|^{z\nu}}, \quad (2)$$

as a function of the distance to the critical point λ_c , the dynamic critical exponent z . and the correlation length critical exponent ν . The constants ξ_0 and τ_0 depend on the microphysics while ν and z depend only on the universality class of the transition. The notions of scale invariance and universality are central in the study of continuous phase transitions. Near the critical point, the characteristic length and the time scales diverge, generating collective phenomena decoupled from the microscopic degrees of freedom. The universality class of the transition obeys a power law in the quench rate, with the exponent given by a combination of the critical exponents of the transition. The same critical exponents will be associated with systems in the same universality class.

In this work, we consider a reduced distance parameter ε defined as

$$\varepsilon = \frac{\lambda_c - \lambda}{\lambda_c}, \quad (3)$$

As $\varepsilon(t)$ varies from $\varepsilon(t) < 0$ to $\varepsilon(t) > 0$, the KZM dynamics takes three stages: adiabatic, nearly frozen, and adiabatic again. When the system crosses the critical point, the phase transition will follow a spontaneous symmetry breaking throughout a change in dynamics from a high-symmetry phase defined by $\varepsilon < 0$ to a degenerate vacuum manifold for $\varepsilon > 0$.

If the system undergoes a linear quench symmetric around the critical point at $t = 0$

$$\lambda(t) = \lambda_c [1 - \varepsilon(t)] \quad (4)$$

the reduced parameter is dependent on the quench time τ_Q and varies linearly in time in $t \in [-\tau_Q, \tau_Q]$

$$\varepsilon(t) = \frac{t}{\tau_Q}. \quad (5)$$

When the equilibrium relaxation time is small enough and far from reaching the critical point $|\lambda| \ll \lambda_c$ following a quench (5), the system behaves adiabatic. Near $\varepsilon(t) = 0$, the divergence of the equilibrium relaxation time causes the system to slow down almost close to freezing, not being able to adjust to the changes of $\varepsilon(t)$. The dynamical evolution of the system does not stop and the order parameter will still continue to evolve locally, but ceasing to follow its global equilibrium value. Therefore, the local thermodynamic equilibrium of the microscopic degrees of freedom in the system can be still maintained. The evolution of the system slows down and stops being adiabatic when the phase transition is crossed at the critical point. The formation of topological defects is a main consequence of the local evolution of the Hamiltonian after crossing the critical point with a delay of \hat{t} and setting up a boundary between the adiabatic and frozen stages. After the initial adiabatic stage, the frozen correlation length generates topological defects and thus the adiabaticity is broken. Consequently, any small change of the control or thermodynamic parameters will lead to non-equilibrium behavior.

The freeze-out time is given by

$$\hat{t} : \left(\tau_0 \tau_Q^{z\nu} \right)^{\frac{1}{1+z\nu}}, \quad (6)$$

The critical point fully controls the non-equilibrium behavior of the system, defining the system trajectory underlying the phase transition in the parameter space. Near the critical point, the equilibrium relaxation time diverges and it can be approximated with the time after crossing the critical point

$$\tau(t) \approx |\varepsilon / \dot{\varepsilon}| = t. \quad (7)$$

The freeze-out behaviour is due to the collective degree of freedom associated with the order parameter not keeping up with any externally imposed changes. In other words, the degrees of freedom associated with the broken symmetry will not follow any change of ε . This sets a delay between the order parameter and the equilibrium point associated with the parameter $\varepsilon \in [-\frac{\hat{\varepsilon}}{\tau_Q}, \frac{\hat{\varepsilon}}{\tau_Q}]$, with

$$\hat{\varepsilon} \equiv |\varepsilon(\hat{t})| : \left(\frac{\tau_0}{\tau_Q} \right)^{\frac{1}{1+z\nu}}. \quad (8)$$

The average size of the regions is defined by the equilibrium correlation length at $\hat{\varepsilon}$, following a power law of \hat{t} when the relaxation time scales as a power law of ε .

$$\hat{\xi} \equiv \xi[\hat{\varepsilon}] = \xi_0 \left(\frac{\tau_Q}{\tau_0} \right)^{\frac{\nu}{1+z\nu}}. \quad (9)$$

If D and d are the dimensions of the space and of the defects, the density of topological defects can be calculated from the value of $\hat{\xi}$

$$n : \frac{\hat{\xi}^d}{\hat{\xi}^D} = \frac{1}{\xi_0^{D-d}} \left(\frac{\tau_0}{\tau_Q} \right)^{(D-d)\frac{\nu}{1+z\nu}}. \quad (10)$$

3. Results

In the following, we investigate the main features of the system's state and its dynamical behavior after a quench and verify the KZM scaling mechanism for zero temperature, by employing powerful numerical tools such as Matrix Product States and Tree Tensor Networks. We analyze the out-of-equilibrium dynamics scenario in the one-dimensional Bose–Hubbard model at zero temperature. We use the Time-Evolving Block Decimation (TEBD) algorithm and use a Suzuki-Trotter decomposition of the Hamiltonian at second order. More specifically, the system is undergoing a linear-ramp quench in the hopping strength J across the second order quantum phase transition, starting from zero temperature. The time evolution of the of the quantum many-body state is here analyzed, starting from the equilibrium state ρ_0 of the Hamiltonian H , which is time-dependent through a linear ramp in the hopping strength

$$J(t) = \frac{2J_c}{\tau_Q} t + J_c, \quad (11)$$

where $J = 0$, and $\mu = 1/2$. If we compare the system's internal relaxation timescale $\tau_R(t)$ with the external driving timescale $\tau_D(t)$, the dynamics splits into two stages: an adiabatic stage for $\tau_R(t) < \tau_D(t)$, and a sudden stage for $\tau_R(t) > \tau_D(t)$. The system's dynamics changes from adiabatic to sudden during the “freeze-out time” \hat{t} . KZM scaling is present if the properties of the system after the quench are dependent on the instantaneous ground state at $\hat{J} = J(\hat{t})$.

Nevertheless, the Hamiltonian is symmetric around the critical point J_c with $J(0) = J_c$ and $J(-\tau_Q/2) = 0$. As the total particle number N is a constant of motion, we therefore have $[H(t), \sum_{j=1}^L n_j] = 0$. Specifically, at zero temperature, ρ_0 is the pure state composed of the perfect Mott insulator state $|\Psi\rangle$ with filling one, i.e. $|\Psi\rangle = |1\rangle_1 \dots |1\rangle_L$, while at finite temperature $\rho_0 = e^{-\beta H_0} / \text{Tr}[e^{-\beta H_0}]$. The initial state ρ_0 is evolved via unitary time evolution $\dot{\rho} = -i[H(t), \rho]$ in the time interval $t \in [-\tau_Q/2, \tau_Q/2]$ and remains a product state at all times. Here, τ_Q is the quench time, while the coupling term vanishes.

As discussed above, the KZM mechanism predicts that the scaling of the final density of defects as a function of the quench time is determined by a single constant exponent κ . The final correlation length will therefore scale as

$$\xi_{\text{fin}} \propto \tau_Q^\kappa, \quad \text{where} \quad \kappa = \frac{\nu}{1+z\nu}, \quad (12)$$

if at the critical point the equilibrium correlation length diverges with a critical exponent ν and the energy gap ΔE closes with another critical exponent $z\nu$. Analytically, the final correlation takes the form

$$\xi_{\text{fin}}(\tau_Q) = 2\sqrt{J_c} \tau_Q + \mathcal{O}(\tau_Q^2). \quad (13)$$

The exponential scaling of $\xi(J)$ at equilibrium, near the critical point J_c can be approached by fitting the exponentials to the equilibrium quantities with a power-law around around the freeze-out

point \hat{J} , resulting into the “effective” critical exponents ν_{eff} and $[z\nu]_{\text{eff}}$. The scaling from Eq. (12) is now recovered by replacing the exponent κ with an effective exponent $\kappa(\tau_Q)$ at zero temperature:

$$\kappa(\tau_Q) = \frac{\nu_{\text{eff}}(\tau_Q)}{1 + [z\nu]_{\text{eff}}(\tau_Q)}. \quad (14)$$

that depends on \hat{J} and on the quench time τ_Q . We numerically compute the freeze-out times $\hat{t}(\tau_Q)$ and the effective critical exponents ν_{eff} and $[z\nu]_{\text{eff}}$, finding that a KZM scaling of the final defect density is here present. For different values of the quench times τ_Q , three different regimes are distinguished: a sudden quench regime for $\tau_Q \hat{< 2$, where the system is driven by a short impulse of duration τ_Q , the KZM scaling regime, for $2 \lesssim \tau_Q < \tau_U$ (where τ_U is the upper bound for τ_Q and it is due to the finite system size) and a finite-size saturation regime when the system is completely ordered and the final correlation length is saturated due to the finite system size. The KZM scaling of the final defect density occurs after the quench time $\tau_Q \geq 2$, when the driving timescale is not sufficiently fast, as for the case $\tau_Q < 2$, so that the quench will begin to slow down and allow the relaxation timescale to catch up with the changes in the system.

4. Conclusion

In summary, using Tensor Network methods as a simulation tool, we studied the effects induced by the initial conditions in a driving critical dynamics and confirm the validity of KZM mechanism for a quench of a quantum system at zero temperature in the one-dimensional Bose–Hubbard model. Furthermore, by analyzing the scaling of the final correlation length ξ_{fin} after the quench and the nonadiabatic behavior of the “defect measure” as a function of the quench duration τ_Q , we find a non-trivial KZM scaling behaviour, in agreement with the theory.

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