

Nonequilibrium Dynamic Critical Scaling of the Quantum Ising Chain

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We solve for the time-dependent finite-size scaling functions of the one-dimensional transverse-field Ising chain during a linear-in-time ramp of the field through the quantum critical point. We then simulate Mott-insulating bosons in a tilted potential, an experimentally studied system in the same equilibrium universality class, and demonstrate that universality holds for the dynamics as well. We find qualitatively athermal features of the scaling functions, such as negative spin correlations, and we show that they should be robustly observable within present cold atom experiments.

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The Kibble-Zurek (KZ) mechanism describes the dynamics of a system as it is ramped across a phase transition at a finite rate. Kibble first introduced this idea to model symmetry breaking during cooling of the early Universe [1]. Later, Zurek showed that condensed matter systems exhibit similar behavior in the context of slowly ramping across the superfluid phase transition in liquid ⁴He [2]. Both proposals looked at ramps from deep in the disordered phase to deep in the ordered phase. Historically, this has been the primary focus of research on the KZ mechanism [3,4], although recent work has explored ramps that end at the critical point [5–7].

However, the scaling theory of the KZ mechanism applies more generally than these two limits. Near the quantum critical point (QCP), observables measured during the ramp are postulated to exhibit universal scaling forms [8,9]. In this Letter, we solve for the scaling functions of excess heat and equal-time spin correlations in the one-dimensional transverse-field Ising (TFI) chain for two scaling directions—time t during the ramp and finite size L —and investigate the qualitative features of these observables. In many cases, the quantum dynamics of a closed nonintegrable quantum system lead to a thermal state. In contrast, we show here that the spin correlation functions are qualitatively different from those of any thermal state. We also find a ramp protocol where the state at long time not only does not thermalize, but also does not dephase to the diagonal (“generalized Gibbs”) ensemble. We provide evidence for the universality of the dynamics by using time-dependent matrix product states (tMPS) to simulate the experimentally realizable, nonintegrable model of Mott insulating bosons in a tilted potential [10,11]. We see that the athermal features of the TFI chain are robust for small systems and discuss the prospects of seeing scaling collapse in present-day experiments.

Transverse-field Ising chain.—The Hamiltonian for the TFI chain on an L -site one-dimensional lattice is

$$H = -J \sum_{j=1}^L [(1 - \lambda)s_j^x + s_j^z s_{j+1}^z], \quad (1)$$

where λ is a tunable transverse magnetic field and $s^{x,z}$ are Pauli matrices with periodic boundary conditions ($s_1 = s_{L+1}$). We work in units where $\hbar = 1$ and $J = 1/2$. This model has a quantum phase transition (QPT) at $\lambda_c = 0$ [12]. In equilibrium, the system is in a disordered paramagnetic (PM) phase for $\lambda < 0$, while for $0 < \lambda < 2$, the system is in a ferromagnetic (FM) phase with two degenerate ordered ground states in the limit $L \rightarrow \infty$.

The Hamiltonian of the TFI chain can be diagonalized by applying a Jordan-Wigner transformation [12,13]:

$$s_j^x = 1 - 2c_j^\dagger c_j, \quad s_j^z = -(c_j + c_j^\dagger) \prod_{m < j} s_m^x, \quad (2)$$

where c_j^\dagger creates a fermion at site j . As the Hamiltonian conserves fermion number modulo 2 and the ground state has an even number of fermions [13], we restrict ourselves to that subspace. Fourier transforming,

$$H = \sum_k \left[(1 - \lambda - \cos k) c_k^\dagger c_k + \frac{\sin k}{2} (c_k^\dagger c_{-k}^\dagger + c_{-k} c_k) \right]. \quad (3)$$

This Hamiltonian can only excite fermions in momentum pairs $(k, -k)$, so we introduce a pseudospin σ corresponding to whether the $(k, -k)$ pair is filled ($\sigma^z = 1$) or unfilled ($\sigma^z = -1$). Then in the sector where all fermions are paired, which contains the ground state, $H = \sum_{k=0}^{\pi} H_k$, where

$$H_k = (1 - \lambda - \cos k) \sigma^z + (\sin k) \sigma^x. \quad (4)$$

Note that H is a free-fermion Hamiltonian, so the TFI chain is integrable.

In a KZ ramp, λ is varied as a function of time near the critical point. For simplicity, we focus primarily on the case of a linear ramp, $\lambda(t) = \nu t$, where ν is the ramp rate

and the QCP is at $\lambda = t = 0$. The ramp begins at $t = -\infty$ deep in the disordered phase, where the wave function is initialized in the ground state of the instantaneous Hamiltonian $H(t = -\infty)$. For an infinite system, the Hamiltonian is gapless at the critical point. Therefore, it is impossible to ramp slowly enough through the QCP to avoid creating excitations and to produce true long range order in the ordered phase.

Near the QCP, critical slowing down tells us that the characteristic time scale $\xi_t \sim \lambda^{-\nu z}$ becomes arbitrarily large, where ν and z are the (positive) correlation length and dynamic critical exponents, respectively. Thus for a nonzero ramp rate, there exists a Kibble time, $-t_K$, at which the lowest momentum modes stop following the ramp adiabatically and become significantly excited. More explicitly,

$$|t_K| = \xi_t[\lambda(|t_K|)] \sim |vt_K|^{-\nu z} \Rightarrow t_K \sim v^{-\nu z/(1+\nu z)}. \quad (5)$$

For the TFI chain, $\nu = z = 1$, so $t_K \sim v^{-1/2}$. One can similarly define a length $\ell_K \sim t_K^{1/z}$ such that t_K and ℓ_K set the characteristic time and length scales for the Kibble-Zurek scaling forms [8,9].

For a KZ ramp of the TFI chain, the wave function $|\psi(t)\rangle$ can be written as a product $|\psi(t)\rangle = \otimes_k |\Psi_k(t)\rangle$, where each mode evolves independently as

$$id|\Psi_k\rangle/dt = H_k(t)|\Psi_k\rangle \\ = [(1 - vt - \cos k)\sigma_k^z + (\sin k)\sigma_k^x]|\Psi_k\rangle. \quad (6)$$

The KZ scaling limit is defined as taking $v \rightarrow 0$ with τ , Λ , and κ constant [8,9], where

$$\tau \equiv tv^{1/2} \sim t/t_K \quad \Lambda \equiv Lv^{1/2} \sim L/\ell_K \\ \kappa \equiv kv^{-1/2} = \frac{2\pi(n+1/2)}{\Lambda} \sim k\ell_K. \quad (7)$$

Here, $n = 0, 1, \dots, (L/2) - 1$ indexes the modes. Note that $L \rightarrow \infty$ in the scaling limit, as $\ell_K \rightarrow \infty$ and Λ is constant. In this KZ scaling limit, Eq. (6) simplifies to

$$id\Psi_\kappa/d\tau = (-\tau\sigma_\kappa^z + \kappa\sigma_\kappa^x)\Psi_\kappa. \quad (8)$$

Each mode $\Psi_\kappa(\tau)$ in Eq. (8) has the form of a Landau-Zener (LZ) equation, which we solve in terms of parabolic cylinder functions [14]. Note that $\Psi_\kappa(\tau)$ is expressed solely in terms of the scaled variables τ and κ .

Observables.—A crude measure of deviation from adiabaticity is the excess heat, defined as

$$Q(t) = \sum_\kappa [\langle \Psi_\kappa(t) | H_\kappa(t) | \Psi_\kappa(t) \rangle - \langle \Psi_\kappa^0(t) | H_\kappa(t) | \Psi_\kappa^0(t) \rangle], \quad (9)$$

where $|\Psi_\kappa^0(t)\rangle$ is the instantaneous ground state of $H_\kappa(t)$. Defining excited state occupancy $p_\kappa^{\text{exc}} = 1 - |\langle \Psi_\kappa^0 | \Psi_\kappa \rangle|^2$ and energy $E_\kappa^{\text{exc}} = 2v^{1/2}\sqrt{\tau^2 + \kappa^2}$, the scaled excess heat density is

$$q(\tau, \Lambda) \equiv \frac{Q(t)}{vL} = \frac{2}{\Lambda} \sum_\kappa p_\kappa^{\text{exc}}(\tau, \Lambda) \sqrt{\tau^2 + \kappa^2}. \quad (10)$$

For the equal time s^z - s^z correlation function, we postulate a nonequilibrium scaling form and check for scaling collapse. The correlation function is defined as $G(x) = \langle s_j^z s_{j+x}^z \rangle$, assuming translation invariance. In equilibrium, s^z has scaling dimension 1/8, so the scaled correlation function is

$$g(\tau, \Lambda, \chi) \equiv G(x, t, L, v)x^{1/4}, \quad (11)$$

where $\chi \equiv xv^{1/2}$. We break up each site into a pair of Majorana fermions [12], such that the correlation function is the Pfaffian of a matrix whose elements are pairwise expectation values of the Majoranas [15]. We evaluate the Pfaffian numerically [16] and find that good scaling collapse occurs for small v [see Fig. 1(a)].

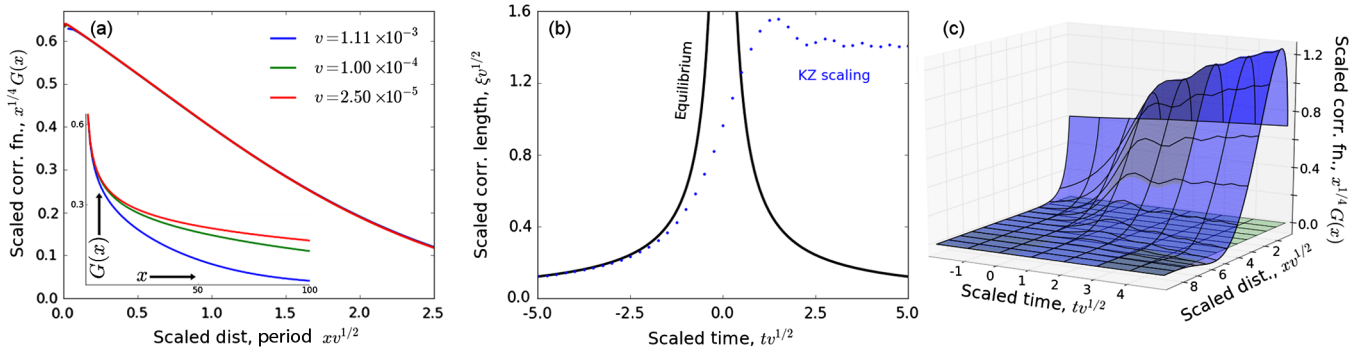


FIG. 1 (color online). (a) Spin-spin correlation function for the TFI chain for a ramp to the QCP ($t = 0$), showing scaling collapse for a wide range of slow ramp rates. The inset shows correlation functions prior to scaling. (b) Scaled correlation length and (c) correlation function as a function of scaled time (b),(c) and distance (c) during the ramp. The KZ correlation length deviates from equilibrium near $tv^{1/2} = -2.5$ and remains finite at the QCP and beyond. We define the correlation length as $\xi v^{1/2} = \sqrt{\int_0^\infty g(\chi)\chi^2 d\chi / \int_0^\infty g(\chi)d\chi}$, where $\chi = xv^{1/2}$. All data in this figure are in the KZ thermodynamic limit, $Lv^{1/2} \gg 1$ (see text).

During the initial part of the ramp ($\tau \ll -1$), the system is very nearly in equilibrium [Figs. 1(b) and 2(a)]. Deep on the FM side of the ramp ($\tau \gg 1$), LZ physics tells us that the excitation probability of mode κ is [14]

$$p_{\kappa}^{\text{exc}} = \exp(-\pi\kappa^2). \quad (12)$$

In between, at finite positive τ , the excitation probability for each mode—given by the LZ equation—oscillates as a function of scaled time before converging to Eq. (12). These oscillations show up in the excess heat [Fig. 2(a)] and the correlation function [Figs. 1(b) and 1(c)].

Finite-size effects enter by opening up a gap at the QCP. In the regime of small scaled size $\Lambda \lesssim 1$, the finite-size gap dominates, the system remains near the ground state, and the solution can be understood perturbatively. On the other hand, in the limit $\Lambda \rightarrow \infty$, the finite-size effects vanish; we will refer to this as the thermodynamic limit of KZ scaling (KZ-TDL). Looking at the correlations right at the QCP [Fig. 2(b)], we see the finite-size crossover from near-equilibrium power-law correlations for $\Lambda = 5$, to a non-equilibrium exponential decay of correlations for $\Lambda = 30$. Similarly, in Fig. 2(a) we see that the scaled excess heat q crosses over from being small at $\Lambda = 5$, where the system is nearly adiabatic, to much larger values at larger Λ .

The TFI chain is integrable, so although a KZ ramp through the critical point creates excitations, the resulting excited states differ markedly from equilibrium thermal states at the same energies. From Eq. (12), we see that at long times the populations of modes with $\kappa^2 < (\log 2)/\pi$ are inverted, i.e., at a negative effective temperature. This leads to qualitatively athermal physics in the scaled correlation function, which goes substantially negative by $\tau = 5$ over a range of scaled distances, as can be seen in Figs. 1(c) and 2(c). This is qualitatively different from any thermal state, which would have a finite correlation length but never negative correlations. Similar behavior has been seen outside the scaling regime for both slow [17] and

instantaneous [18] quenches of the TFI chain and the XY model [19].

Finally, we examine what happens formally as $\tau \rightarrow \infty$ while remaining in the scaling limit; in particular, does the system dephase? For comparison, if one were to stop the ramp at some value λ_f and wait a very long time, the phase differences between modes would increase to the point where the phases are essentially random; this process is known as dephasing. Dephasing in integrable systems is a well-studied problem, and it has been shown that in the long time limit, the observables of the time-evolved pure state approach those of the generalized Gibbs ensemble (GGE; see Ref. [20]), given by removing all phase information from each mode. Here we define the GGE at time τ as the dephased ensemble that one would approach upon freezing the current Hamiltonian and waiting a long time,

$$\rho_{\text{GGE}}(\tau) = \prod_{\kappa} \{ [1 - p_{\kappa}^{\text{exc}}(\tau)] |\Psi_{\kappa}^0(\tau)\rangle \langle \Psi_{\kappa}^0(\tau)| + p_{\kappa}^{\text{exc}}(\tau) |\Psi_{\kappa}^1(\tau)\rangle \langle \Psi_{\kappa}^1(\tau)| \}, \quad (13)$$

where $|\Psi_{\kappa}^1(\tau)\rangle$ is the excited state of mode Hamiltonian H_{κ} . In the limit $\tau \rightarrow \infty$, the mode Hamiltonians asymptote to $H_{\kappa} \propto -\sigma_{\kappa}^z$, so the GGE approaches a fixed value with $|\Psi_{\kappa}^0\rangle \rightarrow |\uparrow\rangle$, $|\Psi_{\kappa}^1\rangle \rightarrow |\downarrow\rangle$, and $p_{\kappa}^{\text{exc}} \rightarrow e^{-\pi\kappa^2}$.

To see if $\tau \rightarrow \infty$ leads to dephasing, we consider the phase difference $\Delta\varphi$ between characteristic modes $\kappa = 0$ and $\kappa = 1$, since excitations are exponentially suppressed for $\kappa \gtrsim 1$. Starting from some time $\tau_i \gg 1$, after which the dynamics is effectively adiabatic, the energy difference ΔE and phase difference $\Delta\varphi$ are

$$\Delta E(\tau) = \sqrt{\tau^2 + 1} - \tau \approx \frac{1}{2\tau}, \quad (14)$$

$$\Delta\varphi = \int_{\tau_i}^{\tau_f} \Delta E(\tau) d\tau \approx \frac{1}{2} \log(\tau_f/\tau_i).$$

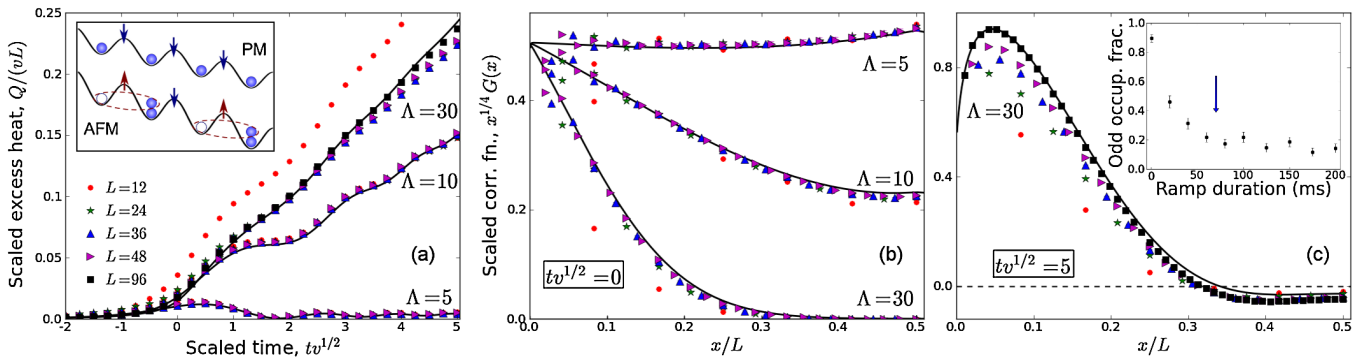


FIG. 2 (color online). Results of tMPS simulations for ramping the experimentally realizable MITP model (see text), which is illustrated in the inset to (a). The data show scaling collapse of MITP (colored dots) to the scaling limit of the TFI chain (black lines) as a function of scaled time $\tau = tv^{1/2}$ (a), scaled system size $\Lambda = Lv^{1/2}$ (a),(b), and scaled length x/L (b),(c) [21]. We have checked that data for $\Lambda = 30$ is near the $\Lambda = \infty$ limit for the TFI model (not shown), although finite-size effects can still be seen in (c). The arrow in the inset to (c) indicates the maximum ramp duration that produces athermal negative correlations in a twelve-site bosonic chain (data from Ref. [11]; see the Supplemental Material [27] for details).

Since $\Delta\varphi \rightarrow \infty$ as $\tau_f \rightarrow \infty$, the phase information between modes is lost in the long time limit, so the observables approach those of the GGE.

We note that, for nonlinear ramps (say cubic ramps, $\lambda \sim t^3$), a similar scaling theory can be written down [8]. Then the above argument again holds, except now

$$\Delta\varphi \approx \int_{\tau_i}^{\tau_f} \frac{1}{2\tau^3} \rightarrow \text{const.} \quad (15)$$

as $\tau_f \rightarrow \infty$, implying that phase information remains and the cubic ramp does not approach the GGE [22]. To summarize, both linear and cubic ramps exhibit athermal behavior, such as negative correlations, which come from the inversion of low-momentum modes, but only the linear ramp dephases to the GGE in the long time limit.

Tilted bosons.—While the TFI chain is a beautiful theoretical model, it is difficult to realize in the lab. However, there have been a number of recent experimental advances with other nonintegrable models in the Ising universality class [11,23,24]. Here we focus on one, the Mott insulator in a tilted potential (MITP), realized experimentally in Ref. [11]. The MITP consists of a one-dimensional lattice containing a Mott insulator with one boson per site. By adding a sufficiently large potential gradient (tilt) δ , the system undergoes a QPT from 1 boson per site to alternately 0 and 2 per site, creating dipoles on every other bond [see Fig. 2(a) inset]. This QCP is in the Ising universality class [10] and can be described by an effective spin Hamiltonian,

$$H_{\text{eff}} = \mathcal{P} \left\{ u \sum_l \left[\delta \frac{S_l^z + 1}{2} - S_l^x \right] \right\} \mathcal{P}, \quad (16)$$

where l labels the bonds, $S^{x,z}$ are Pauli matrices residing on the bonds, and \mathcal{P} is a projector implementing the constraint that no two neighboring bonds are both spin up. The energy scale is set by $u = \sqrt{2}w$, where w is the hopping energy of the lattice bosons; we work in units with $u = 1$. In analogy with the TFI chain, we define the parameters $\lambda = \delta_c - \delta$ and $\nu = \partial_\lambda \lambda$ [21], where $\delta_c \cong -1.31$ is the location of the QCP [10]. The correlation function is given by $G(x) = (-1)^x (\langle S_j^z S_{j+x}^z \rangle - \langle S_j^x \rangle \langle S_{j+x}^x \rangle)$.

We simulate a linear ramp via tMPS, as described in Ref. [7]. Figure 2 shows calculated observables of the MITP model compared to the Ising scaling forms derived earlier. We see clear scaling collapse in all three scaling directions: ramp time t , system size L , and distance x . As expected, simulations do not collapse as well for smaller system sizes. While the dynamic range of the simulations is limited, and the scaling collapse for finite systems is imperfect, we consider our results to be strong numerical evidence for the postulated universality of KZ scaling for systems in the Ising universality class.

We note that, while scaling collapse for the system sizes considered is not perfect at $t\nu^{1/2} = 5$, the correlation function goes negative as predicted from the TFI scaling

function. Therefore, the athermal physics of the KZ ramp is robust against small system sizes and the breaking of integrability, and is a qualitative feature of our model that should be visible experimentally. A major open question is whether such athermal behavior will manifest in KZ ramps near nonintegrable QCPs, where the relatively short-time dynamics of the KZ ramp will be in competition with the long-time expectation of eigenstate thermalization [25].

Finally, we compare our time scales to those of the real experimental system [11]. Using the experimental parameters $w \approx 10$ Hz and $U \approx 400$ Hz, where U is the on-site repulsion, we estimate the ramp rate necessary to see athermal negative spin correlation; our predicted ramp rates are shown in the inset to Fig. 2(c) compared to experimental data from Ref. [11]. Clearly the necessary ramp rates are well within the experimental range [26].

In conclusion, we have solved for the full Kibble-Zurek dynamic scaling forms of the one-dimensional transverse field Ising chain at zero temperature. We provided numerical evidence for the universality of these scaling relations via tMPS simulations of the MITP model. Finally, we determined that the relevant time scales for seeing these effects experimentally is within the reach of current technology. To see full scaling collapse, the experimental system sizes need to be larger, but they should already be sufficient to see qualitatively similar athermal physics.

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