Editors' Suggestion

Universality of Critical Dynamics with Finite Entanglement

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When a system is swept through a quantum critical point, the quantum Kibble-Zurek mechanism makes universal predictions for quantities such as the number and energy of excitations produced. This mechanism is now being used to obtain critical exponents on emerging quantum computers and emulators, which in some cases can be compared to matrix product state (MPS) numerical studies. However, the mechanism is modified when the divergence of entanglement entropy required for a faithful description of many quantum critical points is not fully captured by the experiment or classical calculation. In this Letter, we study how low-energy dynamics of quantum systems near criticality are modified by finite entanglement, using conformally invariant critical points described approximately by a MPS as an example. We derive that the effect of finite entanglement on a Kibble-Zurek process is captured by a dimensionless scaling function of the ratio of two length scales, one determined dynamically and one by the entanglement restriction. Numerically we confirm first that dynamics at finite bond dimension χ is independent of the algorithm chosen, then obtain scaling collapses for sweeps in the transverse field Ising model and the three-state Potts model. Our result establishes the precise role played by entanglement in time-dependent critical phenomena and has direct implications for quantum state preparation and classical simulation of quantum states.

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Introduction.—The long-time dynamics of a many-body quantum system is challenging to study on classical computers even if the system is initialized in a weakly entangled state, as the entanglement entropy will generically grow linearly in time [1–4]. At the same time, this regime of dynamically produced entanglement is of great interest in modern research, as it contains insights into such fundamental questions as how apparently nonreversible thermalization emerges from unitary dynamics in isolated quantum systems [5,6]. The dynamical aspect is particularly important in quantum simulation on current quantum computers, on which preparing a nontrivial ground state is often harder than performing coherent evolution. Yet, compared to static properties, nonequilibrium time evolution is less understood in terms of either conceptual guiding principles or effective methods of calculation.

An exception is the dynamics of a system swept slowly through a quantum critical point, when universal properties are known to emerge in the limit of long times and distances via the quantum Kibble-Zurek (KZ) mechanism. We focus on this mechanism as an example of universal out-of-equilibrium dynamics that is theoretically fundamental and also used in experiments to probe quantum criticality in emerging platforms that maintain quantum coherence well but have difficulty in reaching thermal equilibrium [7]. The modification of quantum criticality by limits on observation time or system size is of renewed interest in light of these new efforts to study such criticality on quantum computers and emulators. Another, more challenging, kind of modification arises from noise or other effects in the system that act to limit quantum entanglement. The goal of the present work is to capture how the quantum Kibble-Zurek mechanism is universally modified in systems with finite entanglement.

Quantum critical points are of particular interest because of their emergent universal properties: their large-scale behavior is insensitive to some "irrelevant" microscopic details and is the same across vast groups of models known as universality classes. However, certain other microscopic perturbations are "relevant" and change the universality class, and indeed finite entanglement will turn out to be such a perturbation. Despite having a degree of robustness to irrelevant perturbations, quantum critical points are also well known to be challenging for computational methods on classical computers, for reasons such as requiring large system sizes that also apply to new efforts on quantum computers. Indeed, finite size can be viewed as a relevant perturbation to criticality, and this insight underlies the successful theory of finite-size scaling [8].

Dynamically, the most straightforward manifestation of universality is the (classical or quantum) Kibble-Zurek scaling. It describes the number and energy of excitations produced in a system that is driven through a second-order phase transition. The scaling of the corresponding density with the drive rate is determined by combinations of standard critical exponents. This behavior is often one of the first phenomena probed on new quantum simulation platforms [9–11], which has also motivated numerical studies of this process [12,13]. We derive forms for the fidelity and excitation energy produced by the sweep based on the existence of two relevant scales: the KZ length ξ_{KZ} arising from falling out of adiabaticity with a nonzero sweep rate, and one ξ_χ arising from the restricted entanglement.

We test the resulting theory using an example of entanglement restriction that is familiar on classical computers: restriction of the bond dimension of a tensor network. The emergence of this length scale ξ_χ is a widely used tool in understanding calculations based on matrix product states (MPS), and as these calculations are among the most used to model the experimental platforms above, we review their use briefly.

MPS originally emerged as the output of the density matrix renormalization group algorithm [14,15], which provides an approximation to the ground states of 1D local Hamiltonians. The efficiency of this algorithm in many cases is underpinned by the area law of entanglement entropy in gapped one-dimensional systems [16] which implies that the exact ground state can be represented efficiently by a MPS [17,18]. Later, MPS inspired the development of other tensor networks, including the multiscale entanglement renormalization ansatz for critical states [19,20] and projected entanglement pair states [21–24]. MPS applications extend beyond ground state properties to include excited states [25–30] and quantum dynamics [30–36].

MPS have also found applications beyond classical simulations of quantum systems. There is a direct mapping between a MPS and certain quantum circuits [37–39]. In such mappings the physical qubits are coupled to some χ-dimensional ancillary system, such as an optical cavity [37], or other qubits [38,39]. Recent work has also demonstrated a mapping between tensor networks and neural networks, the main architecture for machine learning (ML) and artificial intelligence [40,41], allowing for deep learning architectures to be understood from an entanglement perspective [42]. Tensor networks have been successfully used for ML applications, such as image classification [43–49].

For a periodic (or infinite) MPS (iMPS), the expressive power of the ansatz is fully specified by the dimension of the matrices χ, called the bond dimension, which is related to the entanglement entropy of the state [15]; for definitions and details, see the Supplemental Material [50]. However, if the entanglement is unbounded, the existence of an efficient representation of the state with finite χ is no longer guaranteed. This applies whether the MPS is approximating a critical ground state or the entanglement was dynamically generated. Here we consider dynamics where, as in many practical computations, the state is represented by a MPS at finite χ during the full time evolution. We focus on dynamics near a quantum critical point and the goal is to gain insight about properties of the time-evolved state; using the universality of critical behavior, we are able to predict how observables scale with χ and controllably approach the $\chi = \infty$ state from finite-χ data.

We begin with a time evolution protocol known as a Kibble-Zurek sweep [54–57]. We then show that finite χ dynamics is well defined, in that different procedures for time evolution produce the same result in the appropriate limits. A subtlety is that different definitions that all give the exact ground state are no longer equivalent at finite χ, and how algorithms resolve this ambiguity. We then demonstrate our results by examining the transverse-field Ising model (TFIM) and the three-state Potts model, verifying our finite χ scaling hypothesis in detail.

Kibble-Zurek scaling.—We consider an extended quantum system described by a Hamiltonian $H(\lambda)$ with some parameter λ. We further assume that $\lambda = \lambda_0$ corresponds to an isolated quantum critical point. For the correlation length ξ and time τ in the vicinity of the critical point we expect [58]

$$\xi \sim |\lambda - \lambda_0|^{-\nu}, \qquad \tau \sim |\lambda - \lambda_0|^{-z\nu}, \tag{1}$$

where ν and z are the corresponding critical exponents.

Let us now consider the evolution of the system initiated in the ground state (that we assume to be nondegenerate) far away from the critical point with the parameter changing in time as $\lambda(t) = \lambda_0 + vt$. We assume that v is slow compared to the bandwidth and t runs from $-\infty$ to $t_0 > 0$. Far from the critical point the gap is large compared to v and the adiabatic theorem applies. Because the breakdown of adiabaticity only occurs close to the critical point, properties of the resulting state will obey universal scaling laws, the KZ scaling [54–57].

The scaling exponents can be deduced from a simple reasoning. The adiabaticity is lost when $t \approx -\tau$, where τ is determined by Eq. (1); this corresponds to

$$\tau_{\mathrm{KZ}} \sim v^{-[(\nu z)/(1+\nu z)]}, \qquad \xi_{\mathrm{KZ}} \sim v^{-[\nu/(1+\nu z)]}, \tag{2}$$

thus defining the Kibble-Zurek time and length, correspondingly. Since the adiabaticity is restored after $t = \tau$ and we expect the generated exitations to freeze-out and the average density of excitations and energy will be (in one spatial dimension)

$$n_{\mathrm{ex}} \sim 1/\xi_{\mathrm{KZ}} \sim v^{[\nu/(1+z\nu)]}, \tag{3}$$

$$\epsilon_{\mathrm{ex}} \sim 1/\xi_{\mathrm{KZ}}^2 \sim v^{[(2\nu)/(1+z\nu)]}. \tag{4}$$

This scaling has been verified by extensive numerics [59,60] as well as experiments [9,10,61]. There exists also an exact solution for the transverse-field Ising model [51,62].

In Eq. (3), ϵ_{ex} is the energy above the ground state divided by the volume and n_{ex} needs to be defined with care when the particle number is not well defined. We propose to use fidelity density, which is given by

$$f(t) = -\frac{1}{N}\log\left(|\langle\psi(t)|\psi_0\rangle|^2\right), \tag{5}$$

where $|\psi_0\rangle$ is the ground state, $|\psi(t)\rangle$ the time evolved state, and N is the total number of sites in the system. $f(t)$ has the same scaling as we expect for n_{ex} [59,63], and is proportional to it at low densities when the system has a free fermion description, as we explain in Supplemental Material [50].

MPS dynamics and finite bond dimension.—The time evolution of a state under a Hamiltonian $H(t)$ is given by

$$|\psi(t)\rangle = U(t)|\psi(0)\rangle \tag{6}$$

$$U(T) = \mathcal{T}\exp\left(-i\int_0^T dtH(t)\right), \tag{7}$$

where $\mathcal{T}(\cdot)$ is the time ordering operator. If we write $t_n = n\Delta t$, and $T = t_N$, then this is equivalent to writing

$$U(t) = \lim_{N\to\infty}\left[e^{-iH(t_N)\Delta t}\cdots e^{-iH(t_0)\Delta t}\right]. \tag{8}$$

Conceptually, this amounts to treating the Hamiltonian as a piecewise constant over an interval of size Δt, and the exact time evolution is found in the limit that $\Delta t \to 0$. For finite Δt, treating the Hamiltonian as a piecewise constant produces an error of order $\mathcal{O}(\Delta t)$. To implement time evolution using an MPS, if Δt is sufficiently small, it is sufficient to define time evolution for a constant Hamiltonian over a time Δt. We demonstrate in the Supplemental Material [50] that finite χ dynamics is independent of the algorithm used as $\Delta t \to 0$.

Now we turn to how KZ scaling is modified when the state is represented at all times by an MPS with a fixed finite bond dimension χ. The effect of finite bond dimension is to limit the amount of entanglement in the system. And since close to conformal critical points entanglement is related to the correlation length by the celebrated expression [64]

$$S = \frac{c}{6}\log\xi, \tag{9}$$

for fast sweeps, when ξ_{KZ} is small, the effect of χ will be small, whereas for slower sweeps, when ξ_{KZ} is large, the number of excitations will be suppressed compared to Eq. (3).

This situation is similar to the one studied in [12], where the KZ scaling in the TFIM was studied in the presence of a symmetry breaking bias $g_\parallel$ that kept the gap finite at all times during the sweep. It was numerically verified that the effect of $g_\parallel$ could be described by a single length scale $\xi_\parallel = g_\parallel^{-\nu_\parallel}$, where $\nu_\parallel$ is the corresponding critical exponent, and all KZ scaling laws were modified by a scaling function that depended on the ratio $\xi_\parallel/\xi_{\mathrm{KZ}}$. We also expect the scaling behavior to occur for finite system size, in which case the argument of the scaling function would be L/ξ_{KZ} with L, the system size.

Returning to the case of finite bond dimension, we conjecture its effect to be describable by a single length scale ξ_χ. Thus, we expect that the $\chi = \infty$ result is modulated by a dimensionless scaling function, similar to the scaling theory of entanglement entropy [65]. In particular, we expect

$$\mathcal{O}(v,\chi) = \mathcal{O}(v,\chi=\infty)\zeta_{\mathcal{O}}(\xi_{\mathrm{KZ}}/\xi_\chi), \tag{10}$$

where $\zeta_{\mathcal{O}}$ is some scaling function for the observable $\mathcal{O}$. Here, we look at the fidelity density f from Eq. (5) and the excitation energy ϵ_{ex}. The fidelity density f is computed via the largest eigenvalue of the transfer matrix formed by the full contraction of both states (see the Supplemental Material [50]). Both of these quantities require the ground state at finite χ, where equivalent definitions of the $\chi = \infty$ ground state are no longer equivalent. See the Supplemental Material for more details on choosing the relevant finite χ ground state [50].

The length scale ξ_χ has been previously studied for ground state properties and the scaling given by $\xi_\chi \sim \chi^\kappa$ was observed in [66]. The conformal field theory (CFT) entanglement spectrum was used to obtain a form for the exponent [67]

$$\kappa = \frac{6}{c\left(\sqrt{\frac{12}{c}}+1\right)} \tag{11}$$

in surprisingly good agreement with numerical data [66–68]. Looking ahead, we will find that the same critical exponent governs the dynamical problem of Kibble-Zurek scaling.

Numerical verification.—We look at two models in this study. First, the transverse-field Ising model (TFIM), defined by the Hamiltonian

$$H = -J\sum_n \sigma_n^z\sigma_{n+1}^z - g\sum_n \sigma_n^x, \tag{12}$$

where σ_n^i is the ith Pauli matrix at site n. Equation (12) has a Z_2 symmetry $\otimes_i \sigma_i^x$. This system has a quantum phase transition at $g = J$ that separates a disordered phase with a unique GS for $g > J$ and an ordered phase with a twofold degenerate GS for $0 < g < J$. The CFT describing the critical point is the minimal model with $c = 1/2$ and the critical correlation length critical exponent is given by $\nu = 1$ [69]. Thus, for the KZ scaling we expect

$$n_{\mathrm{ex}} \sim v^{1/2}, \qquad \epsilon_{\mathrm{ex}} \sim v. \tag{13}$$

The coupling constants have a υ dependence given by

$$\begin{aligned} J(t) &= 1 + \upsilon t \\ g(t) &= 1 - \upsilon t \end{aligned} \qquad t: -\tfrac{1}{\upsilon} \to 0. \tag{14}$$

The initial coupling is given by $J = 0$, and $g = 2$. The ground state at this point is a simple product state given by $|\psi_0\rangle = |\rightarrow\rangle^{\otimes N}$. We then time evolve this state with the time dependent Hamiltonian using the time-evolution block-decimation (TEBD) algorithm [15,36]. We use a fourth order Trotter decomposition [70], with a timestep of $dt = 0.005$.

We enforce the $\mathbb{Z}_2$ symmetry during the ground state search, and time evolution, producing a $\mathbb{Z}_2$ symmetric state in both cases. For different values of the bond dimension χ, we calculate f and ϵ_{ex}, and show the results in Fig. 1. The black line illustrates the $\chi = \infty$ result. We see that for large υ, the effect of finite bond dimension is minimal, but as we decrease the speed, the deviations become dramatic. The systematic nature of the deviations is a focus of the present work.

In Fig. 2, we show the scaling function collapse assuming the scaling hypothesis in Eq. (10). We expect the scaling hypothesis to be valid for large χ but it already begins to work for $\chi \geq 4$, with the exponent κ specified by Eq. (11).

The second model we explore is the three-state Potts model defined by the Hamiltonian [71]

$$H = -J \sum_n \left(\eta_n^\dagger \eta_{n+1} + \eta_n \eta_{n+1}^\dagger \right) - g \sum_n \left(\tau_n + \tau_n^\dagger \right) \tag{15}$$

$$\eta = \begin{bmatrix} 1 & & \\ & e^{i\frac{2\pi}{3}} & \\ & & e^{-i\frac{2\pi}{3}} \end{bmatrix}, \qquad \tau = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix}. \tag{16}$$

Equation (15) enjoys S_3 symmetry comprised of all permutation of the basis states on all sites. However, we explicitly enforce the only $\mathbb{Z}_3 \subset S_3$ symmetry containing cyclic permutations.

Analogously to the TFIM, at $g = J$ there is a critical point that separates a Z_3 symmetric phase for $g > J$ and a Z_3 ordered phase for $0 < g < J$. The CFT is similarly a minimal model (Z_3 parafermion) with $c = 4/5$ and $\nu = 5/6$ [69]. Accordingly, the KZ scaling is

$$n_{\text{ex}} \sim \upsilon^{5/11}, \qquad \epsilon_{\text{ex}} \sim \upsilon^{10/11}. \tag{17}$$

For the dynamics, we use the same time dependent coupling used for the TFIM, given in Eq. (14). We again use TEBD with a fourth order Trotter decomposition, except with a time step of $dt = 0.01$. The excitation energy, and fidelity density, are qualitatively identical to the TFIM, except with different scaling exponents with υ, and so we relegate the figures to the Supplemental Material [50]. We do show the scaling function collapse in Fig. 3. Again we see a clear collapse of the data, further confirming the scaling hypothesis of Eq. (10).

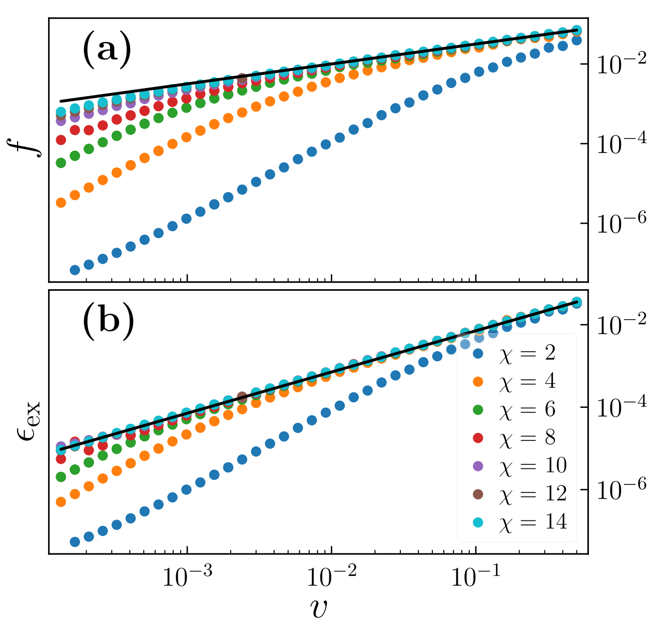

FIG. 1. The fidelity and excitation energy densities after a Kibble-Zurek sweep performed at speed υ for the TFIM. We show the results for different maximum bond dimensions χ. We show a black line illustrating the scaling prediction for $\chi = \infty$.

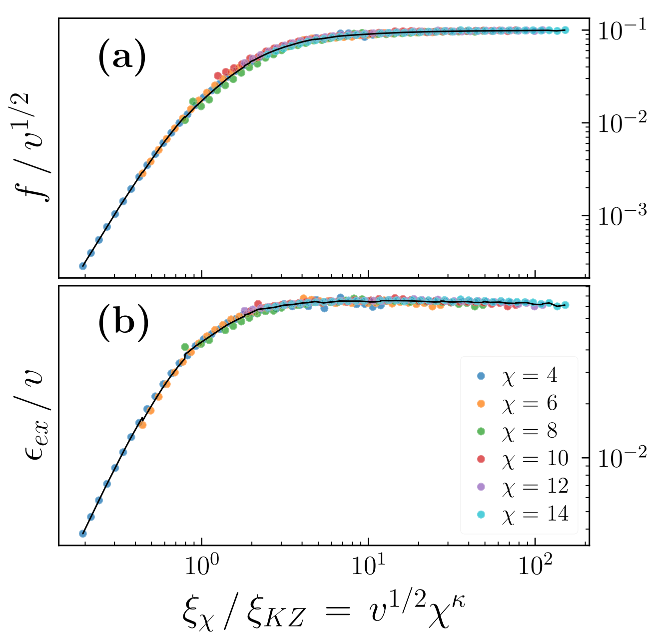

FIG. 2. The scaling function collapse for the fidelity density and excitation energy in the TFIM. The length scale introduced by the bond dimension, ξ_χ, follows a power law with exponent given by Eq. (11), with a central charge of $c = 1/2$.

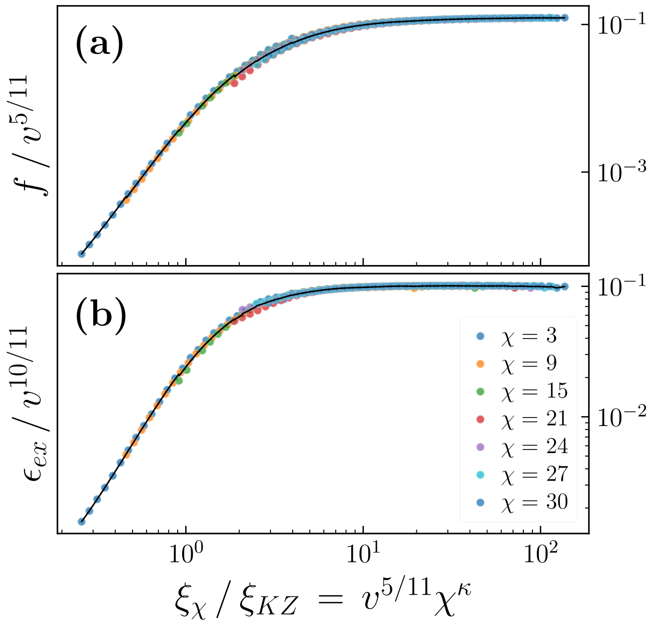

FIG. 3. The scaling function collapse for the fidelity density and excitation energy in the three-state Potts model. The length scale introduced by the bond dimension, ξ_χ is a power law with exponent given by Eq. (11), with a central charge of $c = 4/5$.

Conclusions.—We found that a Kibble-Zurek sweep through a one-dimensional quantum critical point is modified by finite entanglement, i.e., fixed finite bond dimension χ for an iMPS, in a way similar to relevant perturbations of the Hamiltonian, even though finite χ is not equivalent to any local Hamiltonian perturbation. Properly defined, the sweep-induced differences from an adiabatically defined ground state are captured by a universal scaling function that unusually involves both scaling dimensions and central charge. The scaling function involves the ratio of two length scales ξ_{KZ} and ξ_χ and the essential features are independent of the specific implementation of the dynamics, suggesting that the finite-entanglement scaling form for dynamics will have similar utility in practice as the form for ground states, by enabling systematic extrapolation from finite-χ results (see the Supplemental Material for further details [50]).

Whether bond dimension can be treated as a relevant perturbation in an even more general setting, and whether other non-Hamiltonian perturbations to quantum dynamics can similarly be captured by scaling functions, remains an open question. The way matrix product states implement finite entanglement is via the restriction on bond dimension and therefore Schmidt rank: the relevant ground state here was the lowest-energy state within a specified symmetry sector and Schmidt rank. It would be worthwhile to generalize the scaling theory to (pure or mixed) states approximating criticality that arise via other mechanisms that also put a limit on entanglement, such as some nonunitary processes arising from environmental interactions in quantum hardware, and to understand how these approximate states compare to MPS. It would also be interesting to see if our analysis applies beyond Kibble-Zurek scaling to the more general finite-time scaling [72,73]. Lastly, the finite χ scaling of dynamical observables opens up an interesting application of quantum computers in the NISQ era. Since quantum circuits can represent MPSs with a physically relevant bond dimension [37–39], running such simulations at different bond dimensions could enable a novel way to extract the central charge of critical theories. This procedure is well suited for quantum computers, on which unitary dynamics are easily programmed.

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