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Detecting Equilibrium and Dynamical Quantum Phase Transitions in Ising Chains via Out-of-Time-Ordered Correlators

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Out-of-time-ordered (OTO) correlators have developed into a central concept quantifying quantum information transport, information scrambling, and quantum chaos. In this Letter, we show that such an OTO correlator can also be used to dynamically detect equilibrium as well as nonequilibrium phase transitions in Ising chains. We study OTO correlators of an order parameter both in equilibrium and after a quantum quench for different variants of transverse-field Ising models in one dimension, including the integrable one as well as nonintegrable and long-range extensions. We find for all the studied models that the OTO correlator in ground states detects the quantum phase transition. After a quantum quench from a fully polarized state, we observe numerically for the short-range models that the asymptotic long-time value of the OTO correlator signals still the equilibrium critical points and ordered phases. For the long-range extension, the OTO correlator instead determines a dynamical quantum phase transition in the model. We discuss how our findings can be observed in current experiments of trapped ions or Rydberg atoms.

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Introduction—Today, synthetic quantum materials such as ultracold atoms or trapped ions can experimentally access quantum dynamics governed by purely unitary evolution with a negligible coupling to an environment on the relevant timescales [1–4]. This has lead to the observation of quantum dynamical phenomena such as many-body localization [5–8], particle-antiparticle production in the Schwinger model [9], dynamical quantum phase transitions [10–12], or discrete time crystals [13,14]. In many of these phenomena, the propagation of quantum information plays a central role such as for the celebrated logarithmic entanglement growth in many-body localized systems [15,16]. For the quantum formation transport captured by quantum correlations, Lieb-Robinson bounds [17–19] give fundamental constraints, which can be lifted only for long-ranged interacting systems [20] as demonstrated also experimentally [21,22]. Recently, it has been realized that out-of-time-ordered (OTO) correlation functions can capture information propagation beyond quantum correlation spreading [23–32]. In particular, such OTO correlators can diagnose quantum chaos in terms of information scrambling via an exponential growth bounded by a thermal Lyapunov exponent [33].

In this Letter, we show that OTO correlators can also be used to dynamically detect both equilibrium and dynamical quantum phases and the associated quantum critical points. Specifically, we study the OTO correlator dynamics in equilibrium states and after quantum quenches in transverse-field Ising chains with and without long-range couplings. When choosing as the operator in the OTO correlator the order parameter of the underlying transition, we find that the long-time limit serves as a diagnostic tool to detect phases and transitions: In the symmetry-broken phase, the OTO correlator is nonzero and vanishes upon approaching the critical point remaining zero in the full paramagnetic phase. In this way, one can possibly detect quantum criticality in one-dimensional systems that do not exhibit symmetry breaking at nonzero temperatures without preparing the system in the actual ground state, providing a purely dynamical signature of equilibrium quantum phases. We demonstrate our findings for both an integrable as well as nonintegrable version of the one-dimensional transverse-field Ising chain. As a system with a finite-temperature phase transition, we additionally study a long-range transverse-field Ising model where we find that the OTO correlator in equilibrium states correctly captures the equilibrium phases. In the dynamics after a quantum quench, we find that the OTO correlator probes instead a dynamical quantum phase transition of genuine nonequilibrium nature in the system's long-time steady state [12,34]. We also discuss how our results can be observed in current experiments in systems of trapped ions or Rydberg atoms.

OTO correlation functions [35] have been identified as quantities providing insight into quantum chaos and information scrambling [33]. The OTO commutator is defined as

$$C(t) = -\langle [V, W(t)]^2 \rangle \geq 0, \tag{1}$$

where V and W are usually chosen as local Hermitian operators and $W(t) = \exp(iHt)W\exp(-iHt)$ with H the system Hamiltonian. The OTO commutator contains terms of the form $\mathcal{F}(t) = \langle W(t)VW(t)V \rangle$ coined the OTO correlator due to its unconventional temporal structure. These quantities probe the spread of quantum information beyond quantum correlations, in particular signaling the presence of quantum chaos, with a growth bounded by a thermal Lyapunov exponent [33]. Recently, much effort, including experiments [23–30], has been devoted to studying its behavior, with peculiar links to the physics of black holes and random matrix theory [33,36]. Additionally, a simple mesoscopic Sachdev-Ye-Kitaev model [35,37–40] captures many interesting phenomena, including a maximal Lyapunov exponent and entropy characteristic to black holes.

We investigate numerically such OTO correlators in a variety of one-dimensional exhibiting equilibrium and dynamical quantum phase transitions of different kinds. We choose as operators $V = W = \mathcal{M}$ the order parameters $\mathcal{M}$ of the respective transitions in the considered models, which in all of the considered cases is a magnetization

$$\mathcal{M} = \begin{cases} \sigma_n^z & \text{for short-range models,} \\ S^z & \text{for the collective spin model,} \end{cases} \tag{2}$$

where σ_n^z are Pauli matrices and $n = 1, \ldots, N$ with N the total number of lattice sites of the system, and $S^z = N^{-1}\sum_{n=1}^{N}\sigma_n^z$ is the total spin operator. Concretely, we study the dynamics of OTO correlators of the form

$$\mathcal{F}(t) = \langle \mathcal{M}(t)\mathcal{M}\mathcal{M}(t)\mathcal{M} \rangle, \tag{3}$$

with the expectation value $\langle \cdots \rangle = \langle \psi_0 | \cdots | \psi_0 \rangle$. For $|\psi_0\rangle$, we choose two different states. First, we take the respective ground state of the model at the given parameter set in order to probe the equilibrium phase diagram. Second, for the study of the nonequilibrium dynamics, we choose a fully polarized state $|\psi_0\rangle = |\uparrow\uparrow\uparrow\ldots\rangle$, which, on the one hand, can be prepared in experiments of trapped ions or Rydberg atoms with high fidelity [11–13,41–44] and, on the other hand, is well suited to study dynamical quantum phase transitions (DQPTs) in nonequilibrium time evolution with the considered Ising models [11,12,34,45]. We give the details on how to access our theoretical predictions experimentally in the concluding discussion.

Transverse-field Ising chain—Let us start with the paradigmatic model for quantum phase transitions, the 1D transverse-field Ising (TFI) chain [46], whose dynamics has been realized in recent experiments of Rydberg atoms when interactions beyond nearest neighbors can be neglected on the relevant timescales [43,44,47]. Its Hamiltonian with periodic boundary condition reads as

$$H = -J\sum_{n=1}^{N}\sigma_n^z\sigma_{n+1}^z + g\sum_{n=1}^{N}\sigma_n^x, \tag{4}$$

where the σ_n^i's are Pauli matrices and $\sigma_{N+1}^i = \sigma_1^i$ with $i = x, y, z$. This model hosts an equilibrium quantum phase transition (QPT) at $g = J$ separating a paramagnetic phase for $g > J$ from a symmetry-broken phase with nonzero magnetization along the σ^z direction for $g < J$ [46]. For quantum quenches, the system exhibits the appearance of DQPTs with nonanalytic behavior during quantum real-time dynamics whenever the quench crosses the underlying equilibrium QPT [45,48].

The ordered phase can be detected in equilibrium from dynamics by the autocorrelation function $\langle \sigma_n^z(t)\sigma_n^z \rangle$, which takes a nonzero (vanishing) value in the long-time limit in the ferromagnetic (paramagnetic) phase, respectively [46]. However, in the case of a quantum quench, it becomes fully featureless since it vanishes for long times [49,50], irrespective of the Hamiltonian parameters. It would, nevertheless, be advisable to detect both the QPT or DQPT from a dynamical measurement because these are naturally accessible experimentally in quantum simulators. Since the autocorrelation function does not fulfill this job, it looks natural to try its second moment, i.e., $\langle (\sigma_n^z(t)\sigma_n^z)^2 \rangle$, which is nothing but the OTO correlator discussed before.

The model can be mapped onto free fermions such that many correlation functions can be calculated in a simple analytical manner, except for the order parameter σ_n^z [49]. Therefore, we calculate the OTO correlator using numerical methods, such as time evolving block decimation (TEBD) [54] and exact diagonalization (ED). Still, it can be evaluated exactly analytically in certain limiting cases: for $g = 0$, it takes its maximal value 1, while it vanishes in the $J = 0$ limit [55]. In between these two limits, the OTO correlator is expected to interpolate. Whether the transition occurs at the critical point or at some other location is an intriguing question that we investigate in the following.

This we study numerically on finite systems consisting of up to $N = 60$ spins in equilibrium for TEBD and up to 22 spins for ED. The time dependence of Eq. (3) is shown in Fig. 1 for several representative parameter sets both in equilibrium and after a quantum quench, in the ordered and disordered phases. While the real part steady state value of $\mathcal{F}(t)$ depends on whether the time evolving Hamiltonian is in the ordered or disordered region, its imaginary part vanishes identically in the steady state. After a quantum quench, we find that $\mathrm{Im}\mathcal{F}(t) = 0$ such that we focus on the *real* part of the OTO correlator $\mathcal{F}_R(t) = \mathrm{Re}\mathcal{F}(t)$ in the following. $\mathcal{F}_R(t)$ starts from $\mathcal{F}_R(t=0) = 1$ due to the operator identity $(\sigma_n^z)^2 = 1$ and reaches rather quickly a time-independent steady state value before finite size effects start to appear.

Steady state OTO correlator—As obvious from Fig. 1, the steady state value of the OTO correlator can be determined accurately both from the TEBD and ED data

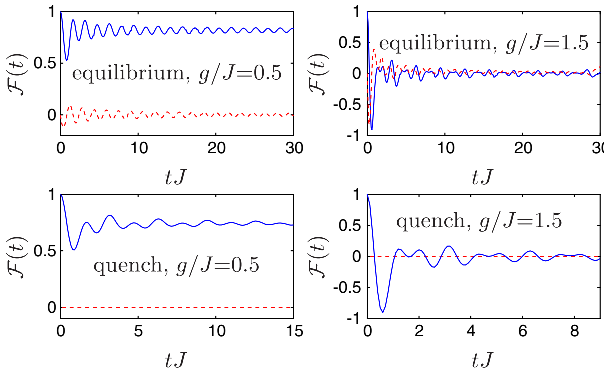

FIG. 1. The representative time evolution of the real (blue solid line) and imaginary (red dashed line) parts of the OTO correlator are shown in equilibrium in the ordered phase with $g/J = 0.5$ and disordered phase with $g/J = 1.5$ from TEBD with $N = 60$. The bottom row visualizes the time evolution following a quench from the fully polarized state from ED with $N = 20$, before finite size effects appear.

by calculating the time average $\bar{\mathcal{F}}$ as the $t \gg 1/J$ limit of $(1/t)\int_0^t \mathcal{F}(t')dt'$, albeit t is still much smaller than the tunneling time (growing exponentially with N) between the almost degenerate ground states for finite N. The results for $\bar{\mathcal{F}}$ obtained in this way are shown in Fig. 2. We find that $\bar{\mathcal{F}}$ is nonzero in the ordered phase and vanishes gradually upon approaching the equilibrium QPT, while it stays zero in the whole disordered paramagnetic phase. This happens not only in equilibrium but also in the case of the quantum quench: the steady state value of the OTO correlator, therefore, serves as a putative order parameter also for the DQPT. Let us stress that this behavior is in stark contrast to the expectation value of $\langle\sigma_n^z(t)\rangle$ or $\langle\sigma_n^z(t)\sigma_n^z\rangle$, which both vanish for long times in the case of a quantum quench [49]. Importantly, one can detect the equilibrium QPT solely [50] by performing a *dynamical* measurement using OTO correlators without ever performing the challenging preparation of the actual ground state but rather doing a quantum quench from an initial condition that can be implemented with high fidelity in current experiments.

The ferromagnetic axial next-nearest-neighbor Ising model.—While the TFI is an integrable model, we now study a nonintegrable extension which is the transverse axial next-nearest-neighbor Ising (ANNNI) model given by [56]

$$H = -J\sum_{n=1}^{N}\sigma_n^z\sigma_{n+1}^z - \Delta\sum_{n=1}^{N}\sigma_n^z\sigma_{n+2}^z + g\sum_{n=1}^{N}\sigma_n^x, \quad (5)$$

where Δ denotes the strength of the second nearest-neighbor interaction. For $\Delta/J = 0.5$, the Ising transition occurs at $g/J \approx 1.6$ [56]. For $\Delta = 0$, the model becomes integrable and reduces to Eq. (4). For $J = 0$, the model again reduces to two identical independent copies of Eq. (4) for the even and odd sites. For these two limiting cases, our previous results hold. For any finite Δ, Eq. (5) becomes nonintegrable [56,57].

We have calculated the OTO correlator of the order parameter using TEBD for the equilibrium case and using ED for the quantum quench. The results are plotted in Fig. 3. The OTO correlator behaves similarly to the integrable case: the imaginary part vanishes for long times in equilibrium and is identically zero after a quench; thus, we focus only on its real part $\mathcal{F}_R$. This takes a finite value in the ferromagnetic phase both in equilibrium or after the quench and vanishes on the paramagnetic side. Therefore, the identification of the OTO correlator as a putative order parameter works ideally for nonintegrable systems as well.

The fully connected transverse-field Ising chain: The Lipkin-Meshkov-Glick model.—Finally, we turn to the Lipkin-Meshkov-Glick (LMG) model [58] describing the fully connected version of Eq. (4). The Hamiltonian

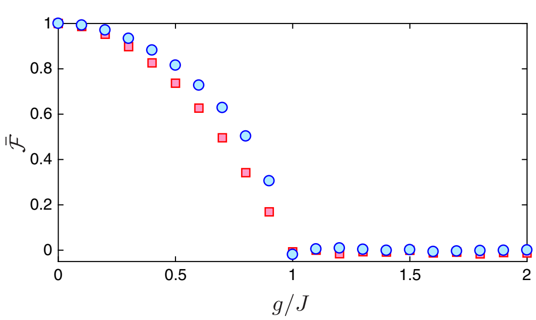

FIG. 2. The long-time average of the order parameter OTO correlator is shown for the TFI chain in equilibrium from TEBD (blue circles) for $N = 60$ and time window $60/J$ and after a quantum quench from a fully polarized state using ED (red squares) for $N = 20$ and time window $20/J$ using numerical data similar to Eq. 1 for several g's.

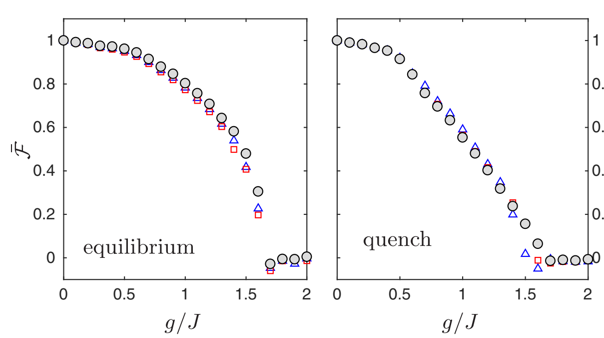

FIG. 3. The long-time average of the order parameter OTO correlator is shown for the nonintegrable TFI chain up until $tJ = 20$ in equilibrium (left) for $N = 20$, 30, and 40 (triangle, square, and circle, respectively) and after a quantum quench from fully polarized state (right) using ED for $N = 12$, 16, and 20 (triangle, square, and circle, respectively), and $\Delta = 0.5$.

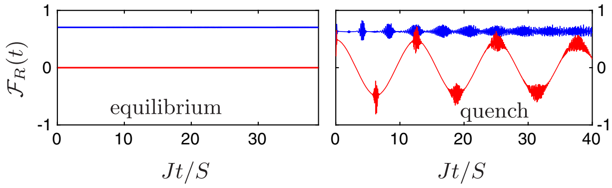

FIG. 4. The representative time evolution of the real part of OTO correlator is shown for the LMG model in equilibrium (left panel) and after a quench (right panel) from the fully polarized state in the ordered phase with $g/J = 0.4$ (blue) and disordered phase with $g/J = 1.2$ (red) for $N = 499$.

of this system can be expressed in terms of the collective spin operators $S^\alpha = \sum_{i=1}^{N} \sigma_i^\alpha/2$, $\alpha = x, y, z$, as

$$H_{\mathrm{LMG}} = -\frac{J}{N}(S^z)^2 + gS^x. \qquad (6)$$

This model exhibits not only a quantum phase transition in the ground state at $g/J = 1$ but also a symmetry-broken phase and respective transition at nonzero temperatures. Consequently, this system allows us to study the dynamics of the OTO correlator in the presence of symmetry breaking at excited energy densities above the ground state, which is absent for the short-range model discussed before and which leads also to a DQPT at $g/J = 1/2$ for quantum quenches when initializing the system in the fully polarized state [12,34]. This DQPT separates a regime of nonzero value of the order parameter S^z in the steady state for $g/J < 1/2$ from a disordered phase for $g/J > 1/2$ where the order parameter vanishes. Importantly, the dynamics of the LMG Hamiltonian can be realized in systems of trapped ions [11,21,22,41,59]. The LMG model is exactly solvable since $[\vec{S}^2, H_{\mathrm{LMG}}] = 0$ such that the Hamiltonian decomposes into disconnected blocks for each of the total spin quantum numbers S. Because of its exact solvability, the system is integrable and not thermalizing. As a consequence, the anticipated DQPT after a quantum quench is not thermal but rather a genuine nonequilibrium transition without an equilibrium counterpart.

In the following, we consider the maximum spin sector $S = N/2$, which also contains the fully polarized initial condition we consider for the quantum quench. As already mentioned in Eq. (2), we calculate the OTO correlator in the LMG model for $\mathcal{M} = S^z/S$. A typical time evolution is depicted in Fig. 4, while the time-averaged value [60] of the OTO correlator is shown in Fig. 5. From the data, one can clearly see that the OTO correlator can both detect the equilibrium as well as dynamical transition. Compared to the previously discussed models, there is, however, an apparent difference. While the equilibrium $\mathcal{F}$ still diagnoses the QPT, the $\mathcal{F}$ after a quantum quench signals the DQPT, suggesting that the detection of the ground-state phase transition from quantum dynamics is limited to the short-range models discussed before. Consequently, we find that the nature of the critical point probed by the OTO correlator depends on the initial condition. Whether it is possible to also detect the thermal transition remains an open question.

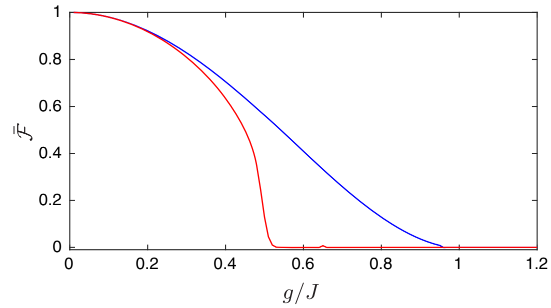

FIG. 5. The long-time average of the order parameter OTO correlator is shown for the LMG model with $N = 1599$ in equilibrium (blue) and after a quantum quench (red) from ED within the time window $20S/J$.

Concluding discussion.—In this Letter, we have shown numerical evidence that OTO correlators can be used to dynamically detect both equilibrium as well as dynamical quantum critical points in one-dimensional short-range and infinite-range transverse-field Ising models.

In addition to serving as an order parameter, our results for the OTO correlation have further ramifications as well. For the operators considered for the TFI and ANNNI models, $C(t) = 2[1 - \mathrm{Re}\mathcal{F}(t)]$ holds. In Refs. [61,62], it was argued that in a suitably chaotic system, the OTO correlator is expected to vanish and the OTO commutator to approach $C(t \to \infty) \approx 2\langle V^2\rangle\langle W^2\rangle$ for any nonzero temperature state. This is exactly what we find in the *disordered* phase of both models for the ground state as well for a quantum quench, as shown in Figs. 2 and 3: the steady state value of the OTO correlator vanishes for $g > J$; therefore, $C(t \to \infty) \to 2$ in the exact same manner as is expected in chaotic systems. In the ordered phase, the situation is, however, different. Both the ground-state and the quantum quench OTO correlators are nonzero. For the considered model, there are two possible explanations for the apparent discrepancy in the conjectured generic long-time dynamics. First, the arguments hold for a generic operator, but the order parameter might not fall under this category. Second, our conclusions hold as long as our time-averaging scheme over a finite time window is suitable and there appears no fundamental change of the OTO correlator dynamics at larger times, for which we also do not find evidence. In this worst-case scenario, our observations would hold over an extended metastable state on intermediate timescales. Summarizing, we find from our study that the OTO correlator dynamics can show unexpected behavior whenever the system exhibits a symmetry-broken phase, which is precisely at the heart of making it a tool to dynamically detect quantum phases.

For the future, it is an interesting question of how the OTO correlator for the order parameter behaves for systems other than the studied Ising chains. Moreover, it is currently unclear what would happen to the OTO correlator for transverse-field Ising models in two and three spatial dimensions, which exhibit symmetry-broken phases at nonzero temperature and in addition are also expected to thermalize in the long-time limit, as opposed to the long-range Ising model studied in this work. Specifically, the OTO correlator either detects the ground state or the thermal transition for which we cannot make a conclusive prediction within our numerics [50].

In the remainder, we now discuss how these observations can be accessed in quantum simulators experimentally. While the considered quantum quench dynamics of the short-range Ising models can be synthesized in Rydberg atoms [43,44], the long-range version can be realized in trapped ions [6,11–13,21,22]. The fully polarized initial condition $|\psi_0\rangle = |\uparrow\uparrow\uparrow\ldots\rangle$ can be realized with high fidelity [11–13,41–44]. Since $|\psi_0\rangle$ is an eigenstate of $\mathcal{M}$ [see Eq. (2)], we only have to consider a reduced quantity $\tilde{\mathcal{F}}(t) = \langle\psi_0|\mathcal{M}(t)\mathcal{M}\mathcal{M}(t)|\psi_0\rangle$. For $\mathcal{M} = \sigma_n^z$, we can reexpress $\tilde{\mathcal{F}}(t) = \langle\psi_t|\mathcal{M}|\psi_t\rangle$ as a conventional expectation value with $|\psi_t\rangle = U^\dagger(t)\exp[i(\pi/2)\sigma_n^z]U(t)|\psi_0\rangle$ where $U(t) = \exp[-iHt]$ using $\exp[i(\pi/2)\sigma_n^z] = i\sigma_n^z$; see, also, Ref. [24]. Consequently, it would be necessary to apply a sequence of unitary transformations implementing (i) a time evolution with the Hamiltonian H, (ii) a local single qubit rotation on spin n, and (iii) a backward time evolution with Hamiltonian $-H$. An additional challenge is that the total simulation time is doubled to $2\times t$ due to forward and backward evolution. Fortunately, clear signatures of the order parameter can be estimated already from the data on times $t \lesssim 5\ \mathrm{J}^{-1}$ (see Fig. 1), which is close to the accessible experimental range [12,43,44].

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