Measuring Entanglement Growth in Quench Dynamics of Bosons in an Optical Lattice

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We discuss a scheme to measure the many-body entanglement growth during quench dynamics with bosonic atoms in optical lattices. By making use of a 1D or 2D setup in which two copies of the same state are prepared, we show how arbitrary order Rényi entropies can be extracted by using tunnel coupling between the copies and measurement of the parity of on-site occupation numbers, as has been performed in recent experiments. We illustrate these ideas for a superfluid-Mott insulator quench in the Bose-Hubbard model, and also for hard-core bosons, and show that the scheme is robust against imperfections in the measurements.

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Entanglement is a basic feature of many-body quantum systems [1] and underlies the complexity of simulating quantum physics on a classical computer [2]. The exponential scaling of resources to represent and propagate a general many-body quantum state on a classical device has motivated the development of quantum simulators [3], and significant progress has been made in building both analog and digital quantum simulators with cold atoms and ions for equilibrium and nonequilibrium dynamics. This is exemplified by quantitative measurement of phase diagrams, studies of quantum phase transitions, and quench dynamics. An outstanding challenge, however, is direct measurement of (potentially large scale) entanglement and monitoring entanglement growth in nonequilibrium dynamics. Below, we address these questions by discussing measurement scenarios for entanglement entropies, using multiple copies of a quantum system and measurements with a quantum gas microscope [4,5]. We illustrate these ideas in the context of quench dynamics of bosons in 1D optical lattices. This example is motivated by recent experiments [6], where quench dynamics were observable for times not accessible to (classical) time-dependent density matrix renormalization group (TDMRG) simulations of Hubbard dynamics [7–10] due to entanglement growth [11–14]. Here the measurement protocol will directly reveal this entanglement growth and simultaneously monitor the purity of the total system state. By comparing copies, these tools will also provide a protocol for the verification of a quantum simulator.

We are interested in quantum dynamics of an (ideally) isolated quantum system as represented by our atomic quantum simulator. In particular, we study a system where we prepare an initial state $|\Psi(0)\rangle$, which evolves with a Hamiltonian H as $|\Psi(t)\rangle = \exp(-iHt/\hbar)|\Psi(0)\rangle$. If the system can be divided into two subsystems A and B and is in a pure state at time t, $\rho = |\Psi\rangle\langle\Psi|$, then the entanglement of the system can be characterized in terms of the entropy of the reduced density matrix, $\rho_A = \mathrm{tr}_B\{\rho\}$. This is commonly computed as the von Neumann entropy $S_{\mathrm{VN}}(\rho) = -\mathrm{tr}\{\rho\log\rho\}$. If A and B are in a product state $|\Psi\rangle = |\Psi_A\rangle \otimes |\Psi_B\rangle$, then ρ_A will also represent a pure state with $\mathrm{tr}\{\rho_A^2\} = 1$, and $S_{\mathrm{VN}}(\rho_A) = 0$. Below, we will discuss measurement of the Rényi entropy of order $n \geq 2$, $S_n(\rho) = \frac{1}{1-n}\log\mathrm{tr}\{\rho^n\}$, which gives quantitative bounds for a variety of measures of entanglement, e.g., the concurrence [15–18], and also $S_{\mathrm{VN}}(\rho)$. For example, we know that $S_{\mathrm{VN}}(\rho)[=\lim_{n\to 1} S_n(\rho)]$, and as $dS_n(\rho)/dn \leq 0$, $S_{\mathrm{VN}}(\rho) \geq S_2(\rho)$. From $d^2S_n/dn^2 \geq 0$, a stronger bound $S_{\mathrm{VN}}(\rho) \geq 2S_2(\rho) - S_3(\rho)$ can be obtained [19] if we measure multiple Rényi entropies.

In order to measure the Rényi entropy $S_n(\rho)$ for a state ρ, we require n copies of the state prepared in parallel and the possibility to implement operations that exchange the n copies [15,20–24]. As shown in Ref. [20], the quantity $\mathrm{tr}\{\rho^n\}$ can be written [20,25] as $\mathrm{tr}\{\rho^n\} = \mathrm{tr}\{V_n\rho^{\otimes n}\}$, where the shift operator on n copies, $V_n|\psi_1\rangle\ldots|\psi_n\rangle = |\psi_n\rangle|\psi_1\rangle\ldots|\psi_{n-1}\rangle$. Therefore, the measurement of the Rényi entropy can be reduced to determining the expectation value $\langle V_n\rangle$ on the n copies. Measurements of inner products can be made in this way by entangling a state with auxiliary qubits or a quantum switch [20,26–28], as has been demonstrated for a few entangled photons [29–31]. In Ref. [22], it was shown that a beam-splitter operation on two copies is sufficient to measure the purity $\mathrm{tr}\{\rho^2\}$ for bosonic systems. Our study of entanglement growth is based on generalizing these techniques to measure Rényi entropies of arbitrary order n. Remarkably, the corresponding experimental tools (controlled tunneling between multiple copies and measurement of on-site occupation numbers modulo n) are now available with single-site addressing in a quantum gas microscope [4,5].

Below, we discuss the protocol to measure $S_n(\rho)$ for arbitrary n and summarize the details of the procedure for the simplest example $n = 2$. We also provide a simplified scheme for hard-core bosons and discuss the robustness of measurements with respect to imperfections. We note throughout that this scheme allows simultaneous measurement of $S_n(\rho)$ for the whole state and for every reduced subsystem (i.e., $\rho = \rho_A$) [32]. Thus, while measurement of the entanglement in this form is based on the assumptions (i) that the initial states for the whole system are pure and (ii) that each evolves under the same Hamiltonian, these assumptions can be checked directly by measuring $S_n(\rho)$ for the whole system. In quench dynamics, these assumptions should be well fulfilled in experiments beginning from low-entropy states [33,34]. Moreover, by monitoring the copies over time and measuring, e.g., $\mathrm{tr}\{\rho_1\rho_2\}$ [20,25], this scheme provides a means to verify a quantum simulator, determining whether the evolution of the copies is coherent and identical on the level of many-body wave functions.

Scheme for arbitrary n.—The procedure to measure the Rényi entropy $S_n(\rho)$ consists of three steps. (i) n identical instances of the many-body state are prepared in parallel (either in n 1D chains or in n planes in 2D). This can be performed, e.g., by beginning from a low-entropy initial state such as a Mott insulator [33,34] and manipulating the lattice potential identically for the two copies, i.e., allowing them to evolve under the same Hamiltonian. In this step, the lattice depth between the copies must remain large so that these are isolated from each other. (ii) We then make the lattice deep within each copy of the state, to prevent tunneling, and perform a discrete Fourier transform U_n^{FT} operation on the copies. If the bosonic annihilation operator for site i in copy $c \in \{1, \ldots, n\}$ is $a_{i,c}$, then

$$U_n^{\mathrm{FT}}\colon\ a_{j,k} \rightarrow \frac{1}{\sqrt{n}} \sum_{l=1}^{n} a_{j,l} e^{i(2\pi/n)(k-1)(l-1)}. \tag{1}$$

This can be achieved by a successive application of tunneling between the copies and shifting the relative potential depths (to produce elements analogous to beam splitters and phase shifters in the optical implementation of this operation [35]). This operation is very simple for small n, as discussed below, and should be performed on the whole system in parallel. (iii) We then perform a site-resolved measurement of the on-site particle number $n_{i,c}$ in each copy, modulo n. We can then determine the measured value of the swap operator $V_n^{\mathcal{R}}$ for all possible subsystems being swapped, $\mathcal{R}$, in parallel (where we note that $\mathcal{R}$ can also denote the whole system), as these commute. The possible measurement outcomes for the swap operations $V_n^{\mathcal{R}}$, $\{e^{ij2\pi/n} | j = 1\ldots n\}$ can then be computed from the number measurements as $\prod_{j\in\mathcal{R}} e^{i2\pi/n \sum_{c=1}^{n} n_{j,c}(c-1)}$. We illustrate this scheme for $n = 2$ below and $n = 3$ in the Supplemental Material [25].

Scheme for n = 2.—As an example, the measurement of the Rényi entropy for $n = 2$ [22] is illustrated in Fig. 1. In step (ii), the Fourier transform for two copies is a beam-splitter operation:

$$a_{i,1} \rightarrow (a_{i,1} + a_{i,2})/\sqrt{2}, \qquad a_{i,2} \rightarrow (a_{i,2} - a_{i,1})/\sqrt{2}. \tag{2}$$

This can be achieved by lowering the barrier between the two copies (e.g., using a superlattice [36]) and allowing the atoms to tunnel from one site to its copy for a time $T = \pi/(4J_{12})$, where J_{12} is the tunneling rate. For this step to work in this form, interactions between atoms have to be turned off during this process, e.g., via a Feshbach resonance. We will show below that this requirement can be relaxed in an alternative method for hard-core bosons. The number measurement modulo 2 in step (iii) is then a parity measurement of the site-resolved occupation number in each site and copy $\{n_{i,c}\}$, exactly as was performed in recent quantum gas microscope experiments [4,5].

The measured value of the swap operator, $V_2^{\mathcal{R}}$, can be computed as $(-1)^{\sum_{i\in\mathcal{R}} n_{i,2}}$, i.e., simply by determining whether the total atom number in block $\mathcal{R}$ of copy 2 after the measurement is even or odd. This process is illustrated in Fig. 1(b) for one measurement instance, and repeating this process allows the expectation value $\langle V_2^{\mathcal{R}}\rangle$ to be computed. To obtain this relationship between the occupation numbers after the beam-splitter operation and $\langle V_2^{\mathcal{R}}\rangle$, we note that each possible measurement outcome $\{n_{i,c}\}$ corresponds to the measurement of one of the two eigenvalues of the (Hermitian) operators $V_2^{\mathcal{R}}$, which are ± 1. This can

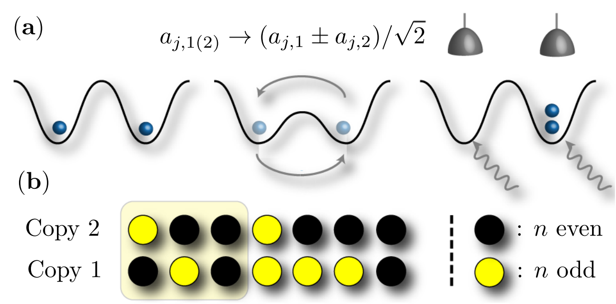

FIG. 1 (color online). (a) Measurement of $n = 2$ Rényi entropy for bosons in an optical lattice. First, two instances of the many-body state are produced (shown here for a single site in a 1D chain or 2D plane). Then tunneling is switched off within each copy, and the barrier between the copies is lowered to realize a beam-splitter operation between the copies. Finally, the parity of the atom number is measured at each site. This measurement is repeated to obtain expectation values for the swap operator V_2, from which the Rényi entropy can be computed (see the text). (b) Example measurement outcome for a single shot on a quantum chain. Here the measurement result for the whole system swap operator $V_2^{\{1,\ldots,7\}}$ is 1, since the total number of particles in copy 2 is even. For the swap of the first three sites $V_2^{\{1,2,3\}}$ is -1, since this number is odd.

be seen as follows: The eigenspaces of $V_2^{\mathcal{R}}$ are the subspaces of the total Hilbert space that are (anti)symmetric with respect to exchange of the two copies, which we denote by $\mathcal{H}_{\mathcal{R}}^{+}$ ($\mathcal{H}_{\mathcal{R}}^{-}$). Since the swap on a subsystem $\mathcal{R}$ can be constructed by local swaps of the sites $j \in \mathcal{R}$, $V^{\{j\}}$, we have $V_2^{\mathcal{R}} = \prod_{j\in\mathcal{R}} V_2^{\{j\}}$. Since all of the $V_2^{\{j\}}$ commute ($[V_2^{\{j\}}, V_2^{\{k\}}] = 0$), we need to consider only a single site. Now, if we denote the annihilation operator for bosons on site i of copy c by $a_{i,c}$, $c \in \{1, 2\}$, the tunneling procedure in step (ii) gives us Eq. (2). This maps the symmetric subspace of the two modes $a_{j,1}$ and $a_{j,2}$ to the subspace of states with an even number of atoms in mode $a_{j,2}$. The antisymmetric subspace is mapped to states with an odd number of bosons in mode $a_{j,2}$. This can be seen by noting that the antisymmetric subspace $\mathcal{H}_j^-$ of the two modes at site j is spanned by the states $\{(a_{j,1}^\dagger - a_{j,2}^\dagger)^{2n+1}(a_{j,1}^\dagger + a_{j,2}^\dagger)^m|\mathrm{vac}\rangle\}$, while the symmetric one $\mathcal{H}_j^+$ is spanned by $\{(a_{j,1}^\dagger - a_{j,2}^\dagger)^{2n}(a_{j,1}^\dagger + a_{j,2}^\dagger)^m|\mathrm{vac}\rangle\}$ (where $n, m = 0, 1, 2, \ldots$). Under the above operation, the first set is mapped onto $\{(a_{j,2}^\dagger)^{2n+1}(a_{j,1}^\dagger)^m|\mathrm{vac}\rangle\}$, i.e., states with an odd number of atoms in $a_{j,2}$, while the second is mapped onto $\{(a_{j,2}^\dagger)^{2n}(a_{j,1}^\dagger)^m|\mathrm{vac}\rangle\}$ with an even number of atoms in $a_{j,2}$. Therefore, the measurement outcome of $V^{\{j\}}$ is $+1$ if $n_{j,2}$ is even and -1 if $n_{j,2}$ is odd.

Example of a Mott insulator-superfluid quench.—We now illustrate the entropy measurement for a quench in the Bose-Hubbard model, where quantum dynamics generates substantial entanglement in a short time [37–39]. In Fig. 2, we plot results obtained via TDMRG calculations from dynamics (in each copy of the system) described by the Bose-Hubbard model ($\hbar \equiv 1$), $H_{\mathrm{BH}} = -J\sum_{\langle i,j\rangle} a_i^\dagger a_j + (U/2)\sum_i a_i^{\dagger 2} a_i^2$, where J is the tunneling rate between neighboring sites $\langle\ldots\rangle$ and U is the on-site interaction strength. We plot both (i) a quench for soft-core bosons from a Mott insulator state with $U/J = 10$ to a superfluid at $U/J = 1$ and (ii) a quench for hard-core bosons $U \to \infty$, where we begin from an initial state with one particle on every second lattice site. Such a state could be produced in a superlattice potential [6] or by using recently demonstrated techniques to directly remove atoms from an initial Mott insulator state [40].

Figure 2(a) shows S_{VN} and S_2 calculated for a bipartite splitting in the center of a small system with 8 particles on 8 lattice sites. In this size of system, we see that the entanglement entropy saturates as the system thermalizes for soft-core bosons [41]. In the hard-core case, the system is integrable, and we see large oscillations in the entanglement entropies instead of thermalization [42,43]. Figure 2(b) shows a comparison between the von Neumann entropy S_{VN} and Rényi entropies S_n (for $n = 2, 3, 4$), after a quench in a larger system with 30 particles on 30 sites. We see rapid growth in the entanglement of two halves of the system, and we note that the Rényi entropies provide relatively good bounds for the von Neumann entropy,

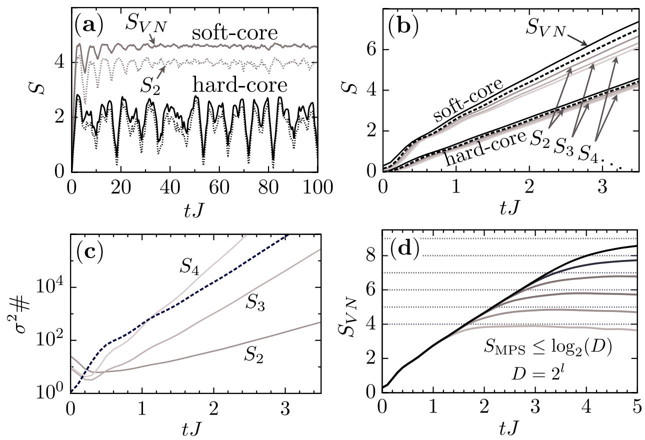

FIG. 2 (color online). Entanglement buildup and measurement, for both (i) soft-core bosons in 1D after a quench from a Mott insulator at $U/J = 10$ to a superfluid at $U/J = 1$ and (ii) hard-core bosons with tunneling J, beginning from an initial state where every second lattice site is occupied. (a) Quenches in small systems with 8 particles on 8 lattice sites, showing von Neumann and Rényi entropies for a bipartite splitting in the center of the system; (b) the same as (a), but for a system of 30 particles on 30 sites, and also including $2S_2 - S_3$ (dotted line). (c) The number of single shot measurements (#) required to determine S_n for the Bose-Hubbard quench in (b) with a relative accuracy σ. For $2S_2 - S_3$, measurements are distributed between (S_2) and (S_3) to minimize the total number. (d) Limitations of TDMRG simulations for the Bose-Hubbard quench based on different bond dimensions D [10], shown here with $D = 2^l$ for $4 \leq l \leq 9$, with corresponding bound $S_{\mathrm{VN}} = l$. Note that we use logarithms to base 2 throughout.

especially if we use the bound $S_{\mathrm{VN}} \geq 2S_2 - S_3$, which is shown as the dashed line in the figure. Figure 2(c) shows the number of single shot measurements required to determine the quantities in Fig. 2(b) with a relative error of σ. We note that, in these larger systems, the TDMRG simulations we use to compute dynamics are limited to simulating short time scales, since the von Neumann entropy increases linearly with time [11,12]. A matrix product state with a bond dimension D [10] is capable of representing a maximum von Neumann entropy up to $\log_2(D)$. In Fig. 2(d), we show the evolution of the entropy as a function of time for $D = 2^l$ with $4 \leq l \leq 9$, showing clearly the different bounds for the entanglement that can be represented. In the case of $D = 512$ we can faithfully simulate time scales only up to $tJ \sim 3$. The simulation times scale $\sim D^3$, and in an experiment, substantially higher entanglement entropies could be generated than are accessible in reasonable time on a classical computer. This could be demonstrated directly by measuring $S_n(\rho)$ in an experiment.

Simplified scheme for hard-core bosons.—The measurement scheme presented above relies on the ability to turn off interactions between the atoms in order to realize the beam-splitter operations, which can be challenging for some atomic species. However, in certain cases this re-

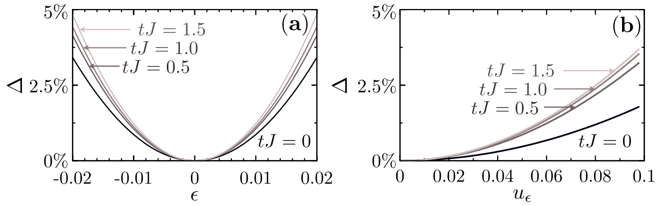

FIG. 3 (color online). Errors $\Delta = [\mathrm{tr}(\rho^2_{a\ldots M}) - \langle \prod_{j=a}^{M} e^{i\pi\hat{n}_j}\rangle_t]/\mathrm{tr}(\rho^2_{a\ldots M})$ that are introduced by an imperfect beam-splitter operation, determined via TDMRG simulation of the Bose-Hubbard quench in Fig. 2(a) and the resulting measurement process. (a) The effect of timing errors, with $T = \pi/(4J_{12}) + \epsilon$; (b) error introduced by a finite interaction strength $u_\epsilon = U_\epsilon/J_{12}$ during the measurement.

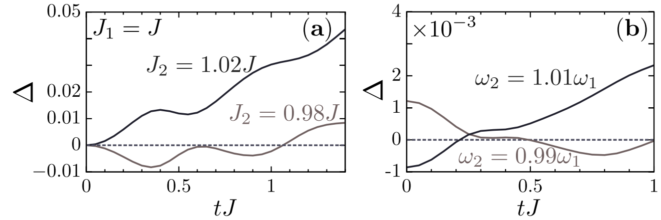

FIG. 4 (color online). Deviations resulting from slightly different evolutions in the two copies, $\Delta = [\mathrm{tr}(\rho^2_{a\ldots M}) - \langle \prod_{j=a}^{M} e^{i\pi\hat{n}_j}\rangle_t]/\mathrm{tr}(\rho^2_{a\ldots M})$. (a) Results for slightly different tunneling amplitudes in each copy after the Mott insulator-superfluid quench from Fig. 2(a). (b) Results for a case where each copy has an additional harmonic trapping potential with $\omega_1 = 2 \times 10J(N/2)^{-2}$ for the first copy, and we otherwise perform the same quench as in (a).

quirement can be relaxed; e.g., in the case of hard-core bosons $U \gg J$, where we have at most one atom per site, the measurement can be performed without switching the interaction strength. For measurement of $S_2(\rho)$, the symmetric subspace at site j, $\mathcal{H}_j^+$, is spanned by $\{|\mathrm{vac}\rangle, (a^\dagger_{j,1} + a^\dagger_{j,2})|\mathrm{vac}\rangle, a^\dagger_{j,1}a^\dagger_{j,2}|\mathrm{vac}\rangle\}$, while the antisymmetric one, $\mathcal{H}_j^-$, is spanned by $(a^\dagger_{j,1} - a^\dagger_{j,2})|\mathrm{vac}\rangle$. Of those four states the tunnel coupling in step (ii) of the measurement scheme affects only states with one particle in total on the copies of the lattice site. The other two states are invariant (either because there are no atoms or because tunneling is suppressed due to the hard-core constraint). Thus we map $\mathcal{H}_j^+ \to \{|\mathrm{vac}\rangle, a^\dagger_{j,1}|\mathrm{vac}\rangle, a^\dagger_{j,1}a^\dagger_{j,2}|\mathrm{vac}\rangle\}$ and $\mathcal{H}_j^- \to a^\dagger_{j,2}|\mathrm{vac}\rangle$ in step (ii). Measurement of the on-site atom number can then be used to directly distinguish between the two eigenspaces of $V_2^{\{j\}}$ and thus determine the measurement result. We extend this to the measurement of $S_3(\rho)$ in the Supplemental Material [25].

Robustness against imperfections.—We now analyze the robustness of the measurements to errors in the measurement steps, especially imperfect implementation of the beam-splitter operations in step (ii). Two main imperfections can occur here, arising from timing errors or residual interactions. In the case of timing errors where $T = \pi/(4J_{12}) + \epsilon/J_{12}$, we can show analytically [25] that the measured value of $\mathrm{tr}\rho^2$ will always be smaller than the actual value by an amount proportional to ϵ^2, thus leaving a clear lower bound. In Fig. 3(a), we plot results obtained from a full TDMRG simulation of the Bose-Hubbard quench from Fig. 2 and the subsequent measurement operation. For timing errors on the order of 1% we find a Δ on the order of 1% which increases slowly with increasing entanglement. In the same calculation, we also consider errors introduced by residual interparticle interactions U_ϵ/J_{12} present during the measurement operation. From Fig. 3(b), we see that even in the case of an interaction of 10% of the beam-splitter tunneling amplitude J_{12} we find resulting errors on the order of only 1% which increase slowly with time.

Nonidentical copies and verification of a quantum simulator.—Another type of imperfection is where the "copies" undergo different dynamics before the measurement process, e.g., due to different Hamiltonians. Such errors are relevant for characterizing the accuracy of the quantum simulator itself, as well as constituting an error in the measurement scheme. In Fig. 4(a), we show results when we have slightly different tunneling amplitudes in each copy after the Bose-Hubbard quench. We find that the error introduced by 2% deviations in J corresponds to a Δ of 1% on a time scale of $tJ \sim 1$, which increases with time. Figure 4(b) shows results from a trapped case, where we begin with slightly different trapping potentials in the individual copies and then perform the same interaction quench from $U/J = 10$ to $U/J = 1$. On a time scale $tJ \sim 1$, errors of 1% lead to deviations on the order of 0.1%. In this case, the quantity that is actually measured is $\mathrm{tr}\{\rho_1\rho_2\}$, where ρ_1 and ρ_2 are the density operators of the different copies. This can be used as a tool to verify the quantum simulator in the case that the evolutions should be identical or to investigate dynamics with the evolution Hamiltonians being set to slightly different values. The latter could be interesting in regimes of the Bose-Hubbard model expected to display signatures of quantum chaos [14,44,45], where the inner product might decay exponentially in analogy with single-particle systems exhibiting quantum chaos [46–48].

Summary.—We have analyzed measurement of Rényi entropies of 1D bosons in an optical lattice during a quench, by using techniques currently available in quantum gas microscope experiments. Such a tool can be used to verify the coherence and accuracy of a 1D and 2D quantum simulator and determine the entanglement growth in a quantum quench, helping the experiments to diagnose regimes where dynamics can be realized that are not accessible to present classical computations.

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quantum systems. We thank D. Abanin and E. Demler for discussions comparing our approaches. P. Z. and H. P. thank the Harvard Physics Department, ITAMP, and the Joint Quantum Institute, University of Maryland, and H. P. thanks the University of Pittsburgh for hospitality. This work was supported in part by the Austrian Science Fund through SFB F40 FOQUS and by a grant from the U.S. Army Research Office with funding from the DARPA OLE program. Computational resources provided by the Center for Simulation and Modeling at the University of Pittsburgh.

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