

Out-of-time-ordered measurements as a probe of quantum dynamics

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Probing the out-of-equilibrium dynamics of quantum matter has gained renewed interest owing to immense experimental progress in artificial quantum systems. Dynamical quantum measures such as the growth of entanglement entropy (EE) and out-of-time ordered correlators (OTOCs) have been shown, theoretically, to provide great insight by exposing subtle quantum features invisible to traditional measures such as mass transport. However, measuring them in experiments requires either identical copies of the system, an ancilla qubit coupled to the whole system, or many measurements on a single copy, thereby making scalability extremely complex and hence, severely limiting their potential. Here, we introduce an alternate quantity – the out-of-time-ordered measurement (OTOM) – which involves measuring a single observable on a single copy of the system, while retaining the distinctive features of the OTOCs. We show, theoretically, that OTOMs are closely related to OTOCs in a doubled system with the same quantum statistical properties as the original system. Using exact diagonalization, we numerically simulate classical mass transport, as well as quantum dynamics through computations of the OTOC, the OTOM, and the EE in quantum spin chain models in various interesting regimes (including chaotic and many-body localized systems). Our results demonstrate that an OTOM can successfully reveal subtle aspects of quantum dynamics hidden to classical measures, and crucially, provide experimental access to them.

I. INTRODUCTION

Quantum phases of matter are generally characterized by the symmetries broken by their ground or finite temperature states, the topological properties of the former, or both. These measures faithfully describe the physics of quantum systems at and near equilibrium. However, they are not suitable for understanding systems far away from equilibrium. In this realm, quantum many body systems are better understood in terms of qualitative features of their dynamics. Classical measures such as mass transport and quantum measures such as entanglement entropy (EE) and out-of-time-correlators (OTOCs) [1–3] have been successful in identifying the dynamics in such systems from a theoretical viewpoint. Seminal examples include the growth of EE after a quench from a high energy state in both chaotic [4] and non-chaotic systems, particularly many-body localized (MBL) systems [5, 6]. The OTOC has also proven very useful for distinguishing between chaotic [7], and localized systems [8–11].

Most experiments, however, are designed to measure time-ordered correlation functions, including classical features such as mass transport. Proposals for adapting them to measure the aforementioned quantum dynamical probes exist; however, they are unfeasible even for modest system sizes, thereby strongly limiting their potential. In particular, current protocols are rooted in tomography and involve measuring every observable in the region of interest to reconstruct the density matrix [12], or entail measuring the overlap of two wavefunctions by creating two identical copies of the same quantum system [13–18], interferometrically using a control qubit that couples to

the entire system [7] or choosing a special initial state whose corresponding projection operator is a simple observable [7, 19]. Due to unfavorable scalability, these approaches appear limiting for a large number of qubits.

In this work, inspired from the OTOCs, we propose an alternative diagnostic, an out-of-time-ordered measurement (OTOM), to probe and distinguish three general classes of quantum statistical phases, namely (i) chaotic (ii) MBL and (iii) Anderson localized (AL). We also comment on (iv) delocalized integrable systems without disorder such as freely propagating particles and Bethe integrable systems (however, we do not study them in detail in this work). All but the first class are integrable. The second and third classes possess local conserved quantities that make them integrable, while integrability in the last class is enforced by non-local conserved quantities.

With regards to experimental accessibility, the OTOM offers several advantages as compared to OTOCs (since it requires only one copy of the system) and tomographic approaches (as it involves only one measurement). Like the OTOCs, it involves reversing the sign of the Hamiltonian to simulate time reversal [20], which has been done in nuclear spin setups [17] and cold atoms experiments [18] with high precision. Within the scope of this work, we are not aiming to be able to understand all the detailed quantum dynamics of the above classes but rather to show that we can reveal them with the new diagnostic. We comment on the experimental feasibility of such a protocol towards the end of the work, as well as on other possible uses of OTOMs.

The plan of the paper is as follows. In Sec. II, we define the new measure and discuss its relationship with

OTOCs. Our analysis of the OTOM will be performed on spin chain models defined in Sec. III, where details of the numerics are also described. Sec. IV contains the results on the different dynamical behaviors of the OTOM in the classes of quantum systems investigated. Finally, Sec. V offers a discussion of these results and comments on the experimental protocols to be used to measure the OTOM.

II. DEFINITIONS OF DYNAMICAL MEASURES

The OTOM is defined as

$$\mathcal{M}(t) = \langle F^\dagger(t) M F(t) \rangle \quad (1)$$

where $F(t) = W^\dagger(t) V^\dagger(0) W(t) V(0)$ (with $W(t) = \exp(iHt) W \exp(-iHt)$) is an out-of-time-ordered (OTO) operator, M is a simple observable, and V and W are local *unitary* operators that commute at $t = 0$ [21]. Thus, $F(0) = \mathbb{1}$ and $\mathcal{M}(0) = \langle M \rangle$. The expectation value is taken in a suitable state ρ for the problem of interest, such as a short-range entangled state, an eigenstate of the Hamiltonian under investigation, or a thermal density matrix. In this work, we choose ρ to be a short-range entangled pure state, $\rho = |\psi\rangle\langle\psi|$.

In contrast, the OTOC is defined as:

$$\mathcal{C}(t) = \langle F(t) \rangle \quad (2)$$

Both the OTOC and the OTOM involve an OTO operator $F(t)$ and therefore have many similar properties. For instance, they have many of the same qualitative features in their time-dependences for dynamics far from equilibrium in the above phases. However, they have important differences, that we will exploit in this work to demonstrate potential advantages of OTOMs in experiments.

Generally, OTOCs can be measured experimentally by applying $F(t)$ on $|\psi\rangle$ to obtain $|\phi(t)\rangle = F(t)|\psi\rangle$. $F(t)$ contains both forward and backward time-propagation operators, $e^{\pm iHt}$; in practice, the latter is implemented in experiments by negating the Hamiltonian. One way to measure a generic OTOC, $\mathcal{C}(t)$, is by measuring the overlap of $|\phi(t)\rangle$ with a second copy of $|\psi\rangle$. Creating two copies of the system, however, becomes prohibitively difficult for large systems. In contrast, OTOM is simply the expectation value of a local observable M in $|\phi(t)\rangle$, and does not require any qubit besides the original system. Note that this procedure is distinct from measuring the dynamical time evolution of a local observable M after a quench; the latter is known to not reveal the dynamics captured by EE/OTOCs.

OTOM vs OTOC: To see how $\mathcal{M}(t)$ is related to $\mathcal{C}(t)$, let us first consider a trace of the form $I = \text{tr}(ABCD)$ for some operators $A \dots D$. Now, any operator can be

thought of as a state in a doubled Hilbert space:

$$A \equiv \sum_{ij} a_{ij} |i\rangle\langle j| \rightarrow \sum_{ij} a_{ij} |i\rangle|j\rangle \equiv |A\rangle \quad (3)$$

$$\langle A| \equiv \left(\sum_{ij} a_{ij} |i\rangle|j\rangle \right)^\dagger = \sum_{ij} a_{ij}^* \langle i|\langle j| \quad (4)$$

If the Hamiltonian of the original system is H , then the doubled system is governed by $\tilde{H} = H \otimes -H$, since kets in the second copy map to bras in the original system. Then, we can think of A and C as states on the two copies, and think of $D \otimes \mathbb{1}$ and $\mathbb{1} \otimes B$ as operators acting on the first and second copy, respectively. Note that this doubling is a purely theoretical construct and is unrelated to the duplication of the experimental system needed for measuring $\mathcal{C}(t)$. Thus, we have

$$I = \text{tr}(ABCD) = \langle A^* | D^T \otimes B | C^T \rangle. \quad (5)$$

Choosing $A = \rho^*$, $B = F^T(t)$, $C = M^T$ and $D = F^*(t)$,

$$\mathcal{M}(t) = \mathcal{M}^*(t) = \text{tr}[\rho^* F^T(t) M^* F^*(t)] \quad (6)$$

$$= \langle \rho | F^\dagger(t) \otimes F^T(t) | M \rangle \quad (7)$$

Equivalently,

$$\mathcal{M}(t) = \left\langle \rho \left| \tilde{V}^\dagger(0) \tilde{W}^\dagger(t) \tilde{V}(0) \tilde{W}(t) \right| M \right\rangle \quad (8)$$

where $\tilde{V} = V^T \otimes V^*$, $\tilde{W} = W^T \otimes W^*$ and time evolution is given by $\tilde{U}(t) = e^{iHt} \otimes e^{-iHt}$, i.e., $\tilde{W}(t) = \tilde{U}(t) \tilde{W}(0) \tilde{U}^\dagger(t)$. Thus, $\mathcal{M}(t)$ is similar to an OTOC constructed from local operators \tilde{V} and \tilde{W} and the Hamiltonian \tilde{H} , albeit with two differences: (i) it is defined on two copies of the same system (it is important to note that the doubled system has the same localization properties as the single copy), and (ii) the matrix element of the OTO operator is evaluated between two different states $|\rho\rangle$ and $|M\rangle$, whereas standard OTOCs are an expectation value of an OTO operator in a given state.

It is not known generally how off-diagonal matrix elements of OTO operators behave in various classes of systems. However, if the two states have a large overlap, we can expect them to qualitatively mimic traditional OTOCs which are expectation values. Thus, we need:

$$|\langle \rho | M \rangle| \equiv \frac{|\text{tr}(\rho M)|}{\sqrt{\text{tr} \rho^2} \sqrt{\text{tr} M^2}} \quad (9)$$

In a Hilbert space of dimension d , the typical magnitude of the overlap between two vectors is $1/\sqrt{d}$. In this paper, we work with a spin-1/2 chain of length L for all our numerical calculations, and choose $M = \frac{1}{L} \sum_i (-1)^i \sigma_i^z$ and $|\psi\rangle = |\uparrow\downarrow\uparrow\downarrow \dots\rangle$. Then $\langle \rho | M \rangle = 1/(\sqrt{L} 2^{L/2}) \gg 1/\sqrt{d}$ where $d = 4^L$ for the doubled system. Thus, $\langle \rho | M \rangle$ is “large” and $\mathcal{M}(t)$ is expected to behave like a traditional OTOC in many ways. Indeed, when $M = \rho = |\psi\rangle\langle\psi|$ (so

that $\langle \rho | M \rangle = 1$), then $\mathcal{M}(t) = |\mathcal{C}(t)|^2$, and we recover the protocol for measuring OTOCs proposed theoretically [7] and implemented experimentally for a small system [19].

We note that an exception occurs when M is a global conserved quantity. In the doubled system, this corresponds to $|M\rangle$ being an eigenstate of \tilde{H} . Then, M is a sum of an extensive number of local terms, and satisfies $[M, H] = 0$, while $[M, W]$ and $[M, V]$ contain $O(1)$ terms each. Thus, W and V can be moved through M in $F(t)$ at the cost of $O(1)$ extra terms, resulting in

$$\frac{\mathcal{M}(t)}{\mathcal{M}(0)} \rightarrow 1 + O(1/\text{volume}) \quad \forall t \quad (10)$$

Thus, the time-dependence of $\mathcal{M}(t)$ is suppressed by the inverse volume of the system when M is a global conserved quantity, so $\mathcal{M}(t)$ stays pinned at its $t = 0$ value for all times in the thermodynamic limit [22]. This behaviour is strikingly different from that of OTOCs in chaotic, MBL and AL phases, where, as we shall see in the following sections, the OTOCs decay exponentially, as a power law, and undergo a short-time evolution before saturating, respectively. However, we will not be concerned with such special choices of M in this work, since global conserved quantities can invariably be either factored out trivially from the analysis, or are too complex to measure experimentally.

Clearly, our specific choices of M , V , W and $|\psi\rangle$ are not necessary for the above qualitative statements as long as V and W are local and unitary, M is the sum of an extensive number of local terms and $\langle \psi | M | \psi \rangle$ is not exponentially small itself. Moreover, we expect these results to generalize to mixed states with short-range entanglement, such as the infinite temperature state, instead of the pure state $|\psi\rangle$, and to extend to other choices of operators and states in generic quantum systems.

III. MODEL AND METHODS

To probe various dynamical behaviors, we consider the spin-1/2 XXZ chain in a random magnetic field:

$$H(\Delta, h) = J \sum_{i=1}^L \sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y + \Delta \sigma_i^z \sigma_{i+1}^z - \sum_i h_i \sigma_i^z$$

We use open boundary conditions and set $J = 1$. The random fields h_i are taken from a box distribution $[-h, h]$. This model offers the advantage of testing different regimes based on the values of its parameters. The special value $\Delta = 0$ corresponds to a free-fermion model. In presence of disorder, this model is celebrated to host a MBL phase at large enough disorder $h > h_c$ for $\Delta \neq 0$, while the low-disorder phase $h \lesssim h_c$ is an ergodic, non-integrable, system. In the Heisenberg case ($\Delta = 1$), the critical disorder is estimated to be $h_c \simeq 7.5$

(for eigenstates near the middle of the spectrum) [23]. When $\Delta = 0$, the model maps to an Anderson-model which is in a localized phase for any $h \neq 0$.

We choose the OTOM operator $M = \frac{1}{L} \sum_i (-1)^i \sigma_i^z$ (staggered magnetization), and the initial state $|\psi\rangle$ as $|\uparrow\downarrow\uparrow\downarrow \dots\rangle$ for all the numerical simulations. We use Pauli spin operators for the local unitary operators, typically $V = \sigma_i^x, W = \sigma_j^x$ or $V = \sigma_i^z, W = \sigma_j^z$.

In the numerics, we use full diagonalization in the $\sigma^z = \sum_i \sigma_i^z = 0$ sector (as σ^z commutes with $H(\Delta, h)$) on chains of length up to $L = 16$, to probe very long time scales. In some cases, we also checked our results on larger systems using a Krylov propagation technique [24], albeit on smaller time-scales. We average quantities over 200 to 1000 disorder realizations for each parameter set. All times are measured in units of $1/J$, which is set to 1.

The OTOM $\mathcal{M}(t)$, being an expectation value of an observable, is real, while the OTOC is in general a complex number. There are cases however where its imaginary part vanishes (for our choice of the initial state, this happens for $V = \sigma_i^z, W = \sigma_j^z$). When the OTOC is complex, we average its modulus $|\mathcal{C}(t)|$ over disorder, while we average over its real part when it is purely real.

Besides these out-of-time order measurements, to highlight the difference between quantum and classical measures, we study two properties of the time-evolved state $|\psi(t)\rangle = \exp(-iHt)|\psi\rangle$: the time-ordered spin imbalance $\mathcal{I}(t) = \langle \psi(t) | M | \psi(t) \rangle$ and the half-system EE, $S(t) = \text{tr}(\rho_A(t) \ln \rho_A(t))$, where $\rho_A(t) = \text{tr}_{\bar{A}} |\psi(t)\rangle \langle \psi(t)|$ is the reduced density matrix obtained by tracing out the degrees of freedom in the other half part \bar{A} of the system.

IV. NUMERICAL RESULTS

A. Local mass transport (imbalance)

In ergodic systems, we expect local densities to relax exponentially fast, as a spin density was shown to do when starting from a classical staggered state [25]. In contrast, this relaxation is incomplete in localized systems, and the spin density settles to a non-zero value both in the presence and the absence of interactions. Fig. 1 shows results for the dynamics of the imbalance $\mathcal{I}(t)$ in three different regimes of the XXZ chain. Mass transport is measured experimentally in a number of systems, and is often taken as a probe of local thermalization [26–28].

B. Quantum phase dynamics

This section contains numerical results for the time evolution of the above measures for a non-integrable system with chaotic transport and for MBL/AL systems with absent particle transport. These examples are chosen to illustrate the important features of both classical

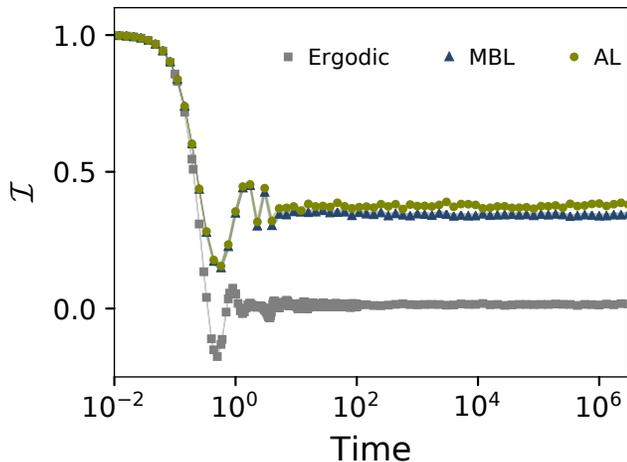


FIG. 1. **Local mass transport:** Imbalance \mathcal{I} (with respect to Néel state) after a quench versus time (log scale), for a $L = 16$ spin chain in three different regimes: AL (for $\Delta = 0, h = 5$), MBL ($\Delta = 0.2, h = 5$) and ergodic ($\Delta = 1, h = 0.5$).

and quantum dynamics. In each case, it appears that the OTOM can reveal the underlying quantum dynamics.

1. Ergodic systems

In a non-integrable system with mass transport (spin transport in the spin chains considered), we expect time-ordered local observables to quickly relax to their long-time expectations values, which is zero in the case of the imbalance \mathcal{I} . At the same time, the OTOCs are also expected to relax exponentially quickly to zero [3], and we anticipate the same for the OTOM. This is indeed what we find, as shown in Fig. 2. As shown in the figure, all operators relax rapidly to zero within a few spin-flip times, and this holds for different choices of the local operators V and W for the OTOC/OTOM. We note that in such a system, the EE grows very fast (ballistically) and saturates to a volume law in the subsystem size [4].

2. Localized systems

Perhaps the clearest distinction of quantum phase dynamics can be observed in dynamics of localized systems. Localization prohibits particle/spin transport completely [29, 30]. Upon performing a quench of the Hamiltonian, it results in a local memory of initial density whether or not interactions are present in the system (see Fig. 1). However, non-local quantities such as EE show distinct behaviors in the presence or absence of interactions due to the involved decoherence (entanglement) of the particle phases between nearby sites [5, 6, 31]. OTOCs readily capture this nature of

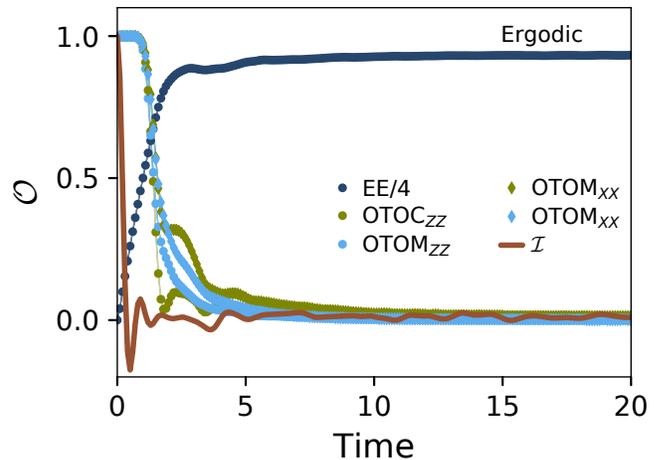


FIG. 2. **Dynamics in a chaotic system:** The OTOC $|\mathcal{C}(t)|$ as well as the OTOM $|\mathcal{M}(t)|$ relax to zero within a couple of tunneling times, the time-ordered imbalance $\mathcal{I}(t)$ vanishes even faster, and the EE $S(t)$ very rapidly saturates to an extensive value. For the OTOC/OTOMs, two sets of results are displayed using different local unitary operators: the OTOM/OTOC denoted XX (ZZ) correspond to $V = \sigma_5^x, W = \sigma_{12}^x$ ($V = \sigma_5^z, W = \sigma_{12}^z$). Other parameters are $L = 16, h = 0.5, \Delta = 1$. Note the linear time scale, as well as the scaling factor for the EE.

the quantum dynamics as well [8–11, 32].

For non-interacting AL systems, particle phases do not entangle with one another. The time evolution of the various quantities is shown in Fig. 3. The EE shows no further time dynamics after an initial increase (due to a finite localization length). Such quickly saturating behavior and absence of dynamics at longer times can also be captured by OTOCs [8–11]. They equal unity in the absence of any time evolution (by definition), and deviate only very slightly from this value with time. More precisely, while their exact time dependence depends on the local spins perturbed by the operators V and W and the strength of the disorder, importantly, they show no time dynamics after an initial resettling (of the order of 50 tunneling times for the parameters of Fig. 3), strongly resembling the dynamics of EE. The time evolution of OTOM for an AL system also displays the same qualitative features: a tiny reduction from unity and no marked time dependence, even up to very long times. This, thus, also provides evidence for the absence of further quantum phase dynamics in such systems, similar to the analysis of the dynamics of entanglement (a non-local probe). The absence of decay is a generic feature, as can be observed for different choices of local operators V and W in Fig. 3. However, one may also argue that the same kind of information is carried by the (absence of) dynamics in a time-ordered quantity such as the normal imbalance (also displayed in Fig. 3), a very local ‘classical’ probe. Hence, to clearly show that the two observables capture

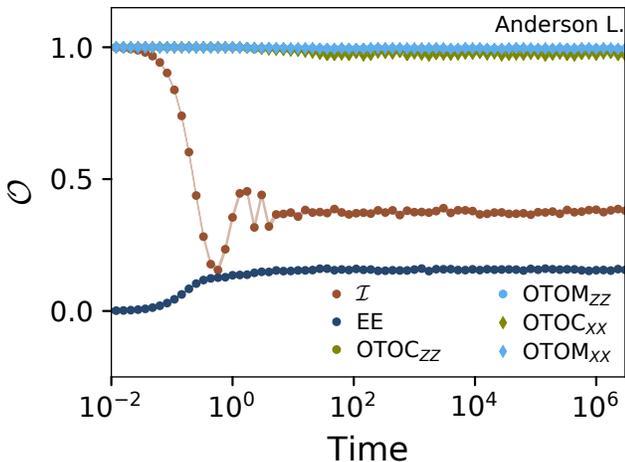


FIG. 3. **Dynamics in an Anderson localized system:** The time-ordered imbalance $\mathcal{I}(t)$ relaxes to non-zero value due to absence of transport (same data as Fig. 1) and the OTOC/OTOM are both close to unity and overlapping. At the same time, the EE $S(t)$ quickly saturates to a finite small value. In such a well localized system, there is almost no intermediate dynamics. Parameters for simulations: $L = 16$, $\Delta = 0$, $h = 5$. For the OTOC/OTOM, we consider operators $V = \sigma_5^x$, $W = \sigma_{12}^x$ (denoted as XX) as well as $V = \sigma_5^z$, $W = \sigma_{12}^z$ (denoted as ZZ) – data for these two different choices are not distinguishable on this scale.

qualitatively different information, it is crucial to look at the interacting generalization of AL systems.

The interacting case of MBL systems offers quite a different situation, due to the slow entangling of quantum phases even in the absence of transport. The numerical calculations for this case are shown in Fig. 4. In such systems, the EE indeed shows time dynamics despite the complete absence of transport, featuring a slow logarithmic growth [5, 6, 31] to reach an extensive value (which is smaller than the one reached in the ergodic phase [31]). At the same time, recent results have shown that time dynamics in MBL systems can also be captured by OTOCs, which have been shown to exhibit a slow power-law like relaxation [8–11]. We also find that the OTOM is capable of capturing the time dynamics in the MBL phase: it shows a slow relaxation similar to the OTOC behavior, albeit it does not reach the same long-time value. This can be understood as the long-time limit of the OTOC depends on the overlap of V and W with the local integral of motions inherent to the MBL phase [11] and we consequently expect that the long-time limit of the OTOM depends on analogous overlaps between V , W and M , resulting in different values.

This observation of slow relaxation at intermediate times is in strong contrast with the behavior of the time-ordered imbalance, which again shows no time dynamics at these timescales of slow dephasing.

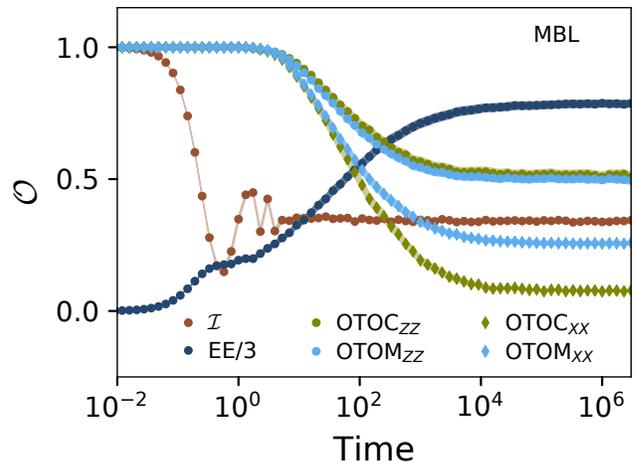


FIG. 4. **Dynamics in a many-body localized system:** Similar to AL, the imbalance \mathcal{I} relaxes to a non-zero value on a relatively short time scale (same data as Fig. 1). On the other hand, the EE $S(t)$ shows a slow logarithmic growth and OTOCs show an apparent slow power-law decay, revealing the quantum phase dynamics at time much longer than the density relaxation time. This slow dynamics is also revealed in OTOMs, which display the same qualitative behavior as OTOCs. Note the lin-log scale for the main panel, the log-log scale for the inset, and the scaling factor for the EE. Parameters for simulations: $L = 16$, $\Delta = 0.2$, $h = 5$. For the OTOC/OTOM, we consider operators $V = \sigma_5^x$, $W = \sigma_{12}^x$ (denoted as XX) and $V = \sigma_5^z$, $W = \sigma_{12}^z$ (denoted as ZZ). The exact long-time limit of OTOC/OTOM depends on the operators chosen for V and W .

V. DISCUSSIONS AND CONCLUSIONS

We have demonstrated that out-of-time ordered measurements OTOMs carry the same information as their correlator counterpart OTOC for three different physical situations: ergodic, AL and MBL systems. We propose a concrete measure which we believe will advance the use of genuinely interesting quantum probes in experiments. Thanks to its scalability, one main application of our probe is to allow experimental access to higher dimensional systems and in particular, to two dimensional systems debated to have an MBL phase [33]. While reversing the sign of the Hamiltonian is a hard task, each term of the Hamiltonian has been sign-reversed in several experiments, including hopping (with a drive), interactions (using Feshbach resonance) and disorder (using a phase shift of the quasi-periodic term). Additionally, this opens the door to measuring quantum dynamics in systems where the initial state cannot be duplicated, such as superconducting qubits, trapped ions and NV-centers.

On the theoretical front, our work naturally opens up several avenues for future studies. Firstly, given that the OTOM is an off-diagonal OTOC in a doubled system, one can ask, “what features of quantum dynamics are

captured by off-diagonal OTOCs that are missed by the usual diagonal OTOCs” and vice versa? Secondly, one can try to exploit the freedom in choosing the OTOM operator M to study aspects of quantum dynamics not studied here. One direct application would be to explore the SYK model [34–37] and the debated Griffiths-phase before the ergodic-MBL transition [38–40]. Another possible continuation is to consider delocalized systems which are integrable, such as systems of free particles or systems soluble by the Bethe ansatz, as they necessarily have non-trivial global conserved quantities (i.e., conserved quantities in addition to trivial ones such as total charge or spin). We noted earlier that OTOMs behave differently from OTOCs when M is chosen to be a global conserved quantity. It would be an interesting extension of our work to compare and contrast OTOCs and OTOMs in these phases in detail. We expect that OTOCs, as well as OTOMs derived from non-conserved quantities would exhibit chaotic (oscillatory) time dependence in Bethe-ansatz soluble (free particle) systems, while OTOMs based on global conserved quantities would show a suppression of any time-independence at all with system size. Finally, unlike ordinary expectation values, OTOMs are able to distinguish between local and global conserved quantities, since only OTOMs based on the latter are expected to remain pinned at their $t = 0$ values in the thermodynamic limit. Naively, local conserved quantities are expected to reduce chaos in a system more than global ones are; OTOMs might be ideally suited for capturing this difference. We leave these open questions for future investigations.

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