

Quantum simulation in the Heisenberg picture: Algorithms and Learning Separations

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Overview. Quantum computers and simulators evade the exponential computational overhead of representing many-body quantum states, yet the information encoded in quantum systems still grows exponentially with system size, making complete classical readout impossible. There is growing recognition that entanglement- [1–4] and randomization-based [5] measurement schemes can dramatically improve measurement efficiency.

However, these approaches have been largely confined to characterizing states. In many settings, the primary goal is to probe dynamical processes directly. Out-of-time-ordered correlators (OTOCs) and multi-point correlators are central diagnostics of many-body dynamics, capturing information scrambling, thermalization, and the spread of quantum correlations [6–17]. Here we develop entanglement- and randomization-enhanced protocols that enable the efficient simultaneous estimation of large families of such quantities.

In the first work of this joint submission, Ref.[18], we introduce a general framework for quantum simulation in the Heisenberg picture using quantum computers. Central to our approach are the vectorization and transfer matrix formalisms, which we exploit to encode Heisenberg operators $O(t) = e^{iHt} O e^{-iHt}$ as quantum states $|O(t)\rangle\rangle$ in a fully structure-preserving manner. As a consequence, *any* task naturally defined in the Heisenberg picture – including sampling from the Pauli distribution of an operator, the computation of (infinite temperature) OTOCs (Out-of-Time-Order Correlators), two-point correlators, operator stabilizer entropies (OSE), local operator entanglement (LOE), and more – can be mapped to tasks in the Schrodinger picture, yielding a set of novel algorithms for their computation.

In the second work of this submission, Ref.[19], we focus on the task of simultaneously learning many correlators at once. Introducing the notion of the *shadow of a Heisenberg operator*, we show how it can be obtained efficiently via randomized measurements with either local or global Clifford measurements. This enables, respectively, the efficient simultaneous estimation of all low-weight OTOCs and all possible two-point correlators. Moreover, treating this as a novel information-theoretic framework to model OTOC-learning protocols, we prove fundamental information-theoretic lower bounds for the task of simultaneously estimating many OTOCs. Considering general OTOC learning protocols with various capabilities such as access to ancillas, adaptivity, and quantum memory (i.e. the ability to entangle multiple copies of the state), we prove lower bounds on certain OTOC learning tasks, which imply both the optimality of our algorithms, and exponential learning separations in several situations.

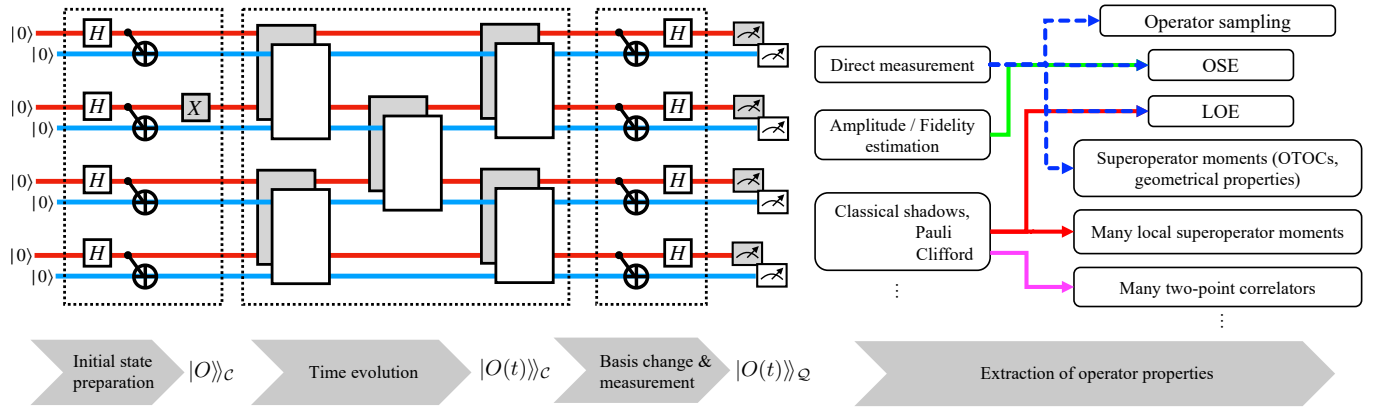


Figure 1: Schematic of our main framework, consisting of preparing and extracting information from $|O(t)\rangle\rangle$.

Framework. Central to our main framework is the vectorization map, which encodes n -qubit Heisenberg operators as $2n$ -qubit quantum states $|O(t)\rangle\rangle$. Given any $O(t) = UO(t=0)U^\dagger$ where U is a unitary, it is defined as the map:

$$O(t) = \sum_{k=1}^{4^n} c_k P_k \longleftrightarrow |O(t)\rangle\rangle \equiv \sum_{k=1}^{4^n} \frac{c_k}{\sqrt{\sum_i |c_i|^2}} |k\rangle, \quad (1)$$

where $\{P_k\}_{k=1}^{4^n}$ is the n -qubit Pauli basis (or any orthonormal operator basis). Summarized in Fig. (1), our framework consists of preparing, time-evolving, and subsequently extracting information from $|O(t)\rangle\rangle$ via measurements on a quantum computer. We show that samples of $|O(t)\rangle\rangle$ can be prepared efficiently under reasonable conditions. Once this is done, information regarding $O(t)$ can be extracted.

Algorithms. Importantly, the mapping $O(t) \leftrightarrow |O(t)\rangle\rangle$ is an isometric isomorphism, implying that *any* task or property involving Heisenberg operators can be mapped to those involving quantum states (and vice versa). This central observation allows us to propose a plethora of quantum algorithms for the extraction of operatorial properties, summarized in the table below; precise sample complexities of our algorithms are detailed in Sections III~VI of [18].

Properties of $O(t)$	Properties of $ O(t)\rangle\rangle$	Method of extraction
Operator distribution in $\mathcal{Q}$	Probability distribution in computational basis	Measurement in computational basis
OTOCs/statistical moments of self-adjoint superoperator $\mathcal{A}$, $\text{tr}(O(t)\mathcal{A}(O(t)))$	Expectation value of Hermitian transfer matrix $M^{\mathcal{A}}$ of $\mathcal{A}$, $\langle\langle O(t) M^{\mathcal{A}} O(t) \rangle\rangle$	Measurement in eigenbasis of $M^{\mathcal{A}}$ and evaluation of Monte Carlo estimator (Theorem 3, [18])
Operator amplitudes $\text{tr}(Q_k O(t))$ /inner products $\text{tr}(O_1 O_2)$	Amplitude in computational basis / inner product between states	Amplitude/fidelity estimation (Section VI, [18])
Operator Stabilizer Entropy (OSE)	Inverse participation ratio of probability distribution of $ O(t)\rangle\rangle$ in Bell basis	Measurement and fidelity/amplitude estimation (Theorem 1, [18])
Local Operator Entanglement (LOE)	Subsystem entanglement entropy of $ O(t)\rangle\rangle$	Multivariate trace estimation (Theorem 2, [18])
Pauli classical shadow of $O(t)$	Pauli classical shadow of $ O(t)\rangle\rangle$	Random Pauli measurements (Theorem 1, [19])
Clifford classical shadow of $O(t)$	Clifford classical shadow of $ \sigma(O(t))\rangle\rangle$	Random global Clifford measurements (Theorem 2, [19])

Table 1: Properties of $O(t)$, corresponding properties encoded in $|O(t)\rangle\rangle$, and their extraction on quantum computers.

An important subroutine is the ability to directly sample from the *Pauli distribution* of $O(t)$, $p(P_k, O(t)) \propto c_k^2$. Among other uses, it enables the Monte-Carlo estimation of quantities of the form:

$$F(O(t)) = \sum_k p(P_k, O(t)) f(P_k, O(t)) = \mathbb{E}_{k \sim p(P_k, O)} [f(P_k, O(t))], \quad (2)$$

where $f(P_k, O(t)) \in \mathbb{R}$ is a general non-linear function of $O(t)$ and/or P_k . This yields efficient estimators for several key quantities defined in the Heisenberg picture, as long as $f(P_k, O(t))$ can be evaluated efficiently (classically or quantumly), and the estimator variance is bounded. This underlies our algorithms for OTOCs/superoperator expectation values, the OSE, and the LOE. Focusing on OTOCs, we show that exploiting commutativity enables large families of OTOCs to be simultaneously estimated (Theorem 3, [18]). Furthermore, Pauli sampling enables *all* geometrical properties of $O(t)$ – such as its volume, boundary size, velocity, etc. – to be simultaneously extracted.

Furthermore, we introduce the notion of the *shadow of an operator*, which are compressed classical descriptions of $O(t)$ that encode operatorial properties. These are an extension of the framework of classical shadows [5] to the Heisenberg picture that can be constructed efficiently from $|O(t)\rangle\rangle$ via randomized measurements in suitable bases:

Pauli operator shadow. When constructed via local Pauli measurements on $|O(t)\rangle\rangle$, the resulting shadow enables the efficient estimation of all *low-weight OTOCs*, i.e. $\text{tr}(O(t)PO(t)Q)$, where both $P, Q \in \mathcal{P}_n$ are supported non-trivially on a small number of qubits (Theorem 1, [19]).

Clifford operator shadow. When constructed via global Clifford measurements on a close variant of $|O(t)\rangle\rangle$, the resulting shadow enables the efficient estimation of, remarkably, *all* two-point correlators $c_k = \text{tr}(O(t)P_k)$ (Theorem 2, [19]). Stronger than Schrodinger-picture Clifford shadows, this includes the signs of c_k .

Besides yielding novel algorithms for the OSE and LOE, our framework formalizes prior methods for estimating OTOCs [6, 8, 20, 21] via the vectorization and superoperator formalisms, and generalizes them for the simultaneous estimation of many quantities. Our algorithms for two-point correlators complement existing channel learning protocols [4], showing that the ability to query $U^\dagger$ can significantly simplify their simultaneous computation.

Fundamental lower bounds on OTOC learning. Out-of-time-ordered correlators (OTOCs) are widely used probes of quantum chaos and scrambling: much like the classical butterfly effect, they quantify how strongly a small, localized perturbation becomes “amplified” under time evolution, thereby making the dynamics difficult to reverse. In the

standard unitary setting, for a time-evolution operator U and Pauli operators P, Q , the OTOC can be defined as

$$F(U; P, Q) = \frac{1}{d} \text{tr}(U^\dagger Q U P U^\dagger Q U P) = \frac{1}{d} \text{tr}(Q(t) P Q(t) P), \quad (3)$$

where $Q(t) = U^\dagger Q U$ and d is the Hilbert-space dimension.

To model existing protocols for learning OTOCs, we extend this notion beyond closed-system dynamics, by generalizing evolution under U to the (noisy) quantum channel $\mathcal{E}$, and evolution under $U^\dagger$ to the adjoint $\mathcal{E}^*$. Concretely, we consider protocols that learn OTOCs by querying the composite channel $\mathcal{O} \equiv \mathcal{E}^* \circ \tilde{\mathcal{O}} \circ \mathcal{E}$, i.e., implement the channel $\mathcal{E}$, followed by conjugation by some Pauli gate $O(t=0)$ (denoted $\tilde{\mathcal{O}}$), then the adjoint channel $\mathcal{E}^*$. The channel $\mathcal{O}$ can be interpreted as implementing a Loschmidt echo. Importantly, this model captures the vast majority of existing OTOC-learning protocols, such as [6–8, 16, 20–28], and our algorithms above. This information-theoretic framework allows us to prove lower bounds for learning protocols that estimate such OTOCs via oracle access to $\mathcal{O}$.

We first consider the problem of estimating many low-weight OTOCs (i.e. M quantities $\{\text{tr}(P\mathcal{E}(Q)P\mathcal{E}(Q'))\}$, where Q, Q' are Pauli operators of weight- w). This task can be solved by Pauli operator shadows efficiently. This algorithm is in fact optimal among the class of single-copy non-adaptive protocols, due to the following information-theoretic lower bound:

Theorem 1 (Sample complexity lower bound for learning low-weight OTOCs). *Any OTOC learning protocol (without ancillas and quantum memory) based on querying $\mathcal{O}$ to learn M arbitrary weight- w OTOCs require $\Omega(9^w \log(M)/\epsilon^2)$ queries. This scaling is achieved by Pauli operator shadows.*

Next, consider the problem of estimating all $4^n - 1$ diagonal OTOCs $\{\text{tr}(P\mathcal{E}(Q)P\mathcal{E}(Q))\}_{Q \in \mathcal{P}_n \setminus \mathbb{I}}$ to ϵ error with constant success probability. Our first work [18] hinted at the difficulty of this problem with access to only n -qubits, due to the inability to sample from the Pauli distribution of $O(t)$ (Section VIII, [18]). The following result verifies this intuition; we rigorously show an exponential separation in query complexity between protocols with access to only n qubits, versus those with access to $2n$ qubits:

Theorem 2 (Exponential separation in estimating diagonal OTOCs, with vs without ancillas).

- Consider a learning protocol that can query $\mathcal{O}$ on arbitrary n -qubit initial density matrices, with no ancillas, but can access quantum memory and be concatenating and adaptive. Such a protocol requires $\Omega(2^n/\epsilon^2)$ queries to solve the diagonal OTOC estimation problem.
- On the other hand, consider the same class of learning protocols, but with access to n ancillas. There is a such protocol that solves the same problem, using only $\mathcal{O}(n/\epsilon^2)$ queries.

Notably, this separation holds even when adaptivity and quantum memory/concatenation of queries are allowed, illustrating the crucial role of ancillas to close the exponential gap. Indeed, we also show that our algorithm based on Eq. (2) via Pauli-distribution-sampling is optimal (among non-adaptive protocols without quantum memory; [19]), and more generally that the query complexity of this problem using k ancillas is $\Theta(n2^{n-k}/\epsilon^2)$.

Finally, consider the (harder) task of estimating all OTOCs $\{\text{tr}(P\mathcal{E}(Q)P\mathcal{E}(Q'))\}_{Q, Q' \in \mathcal{P}_n \setminus \mathbb{I}}$, including off-diagonal ones (where the operator P appearing in Eq. (3) can differ). Our second result shows that this task exhibits an exponential separation in query complexity between protocols with and without access to quantum memory:

Theorem 3 (Exponential separation in estimating OTOCs, with vs without quantum memory).

- Consider a learning protocol that can query $\mathcal{O}$ on arbitrary initial density matrices (involving any number of ancillas) and can be adaptive, but without quantum memory. Such a protocol requires $\Omega(4^n/\epsilon^2)$ queries to solve the all OTOC estimation problem.
- On the other hand, consider the same class of protocols, but with quantum memory. There is such a protocol that solves the same problem, using $\mathcal{O}(n/\epsilon^4)$ queries.

Punchline. In Ref.[18] we establish a unified framework to probe operator dynamics on quantum hardware via preparing vectorized Heisenberg evolved operators on quantum hardware. This framework can be used to compute ‘operator hydrodynamical’ quantities as summarized in Table 1. In Ref.[19] we introduce the notion of the *shadow of an operator* for computing OTOCs and two-point correlators, and prove their optimality. We further provide exponential learning separations that establish that sampling from the $2n$ -qubit vectorized operator can enjoy exponential separations over standard n -qubit approaches. Together, Refs. [18, 19] open new opportunities for probing operator hydrodynamics, providing new provably more efficient tools for diagnostics of many-body dynamics, capturing information scrambling, thermalization, and the spread of quantum correlations.

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