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Learning many-body Hamiltonians with Heisenberg-limited scaling

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Learning a many-body Hamiltonian from its dynamics is a fundamental problem in physics. In this work, we propose the first algorithm to achieve the Heisenberg limit for learning an interacting N -qubit local Hamiltonian. After a total evolution time of $\mathcal{O}(\epsilon^{-1})$, the proposed algorithm can efficiently estimate any parameter in the N -qubit Hamiltonian to ϵ -error with high probability. Our algorithm uses ideas from quantum simulation to decouple the unknown N -qubit Hamiltonian H into noninteracting patches and learns H using a quantum-enhanced divide-and-conquer approach. The proposed algorithm is robust against state preparation and measurement error, does not require eigenstates or thermal states, and only uses $\text{polylog}(\epsilon^{-1})$ experiments. In contrast, the best existing algorithms require $\mathcal{O}(\epsilon^{-2})$ experiments and total evolution time. We prove a matching lower bound to establish the asymptotic optimality of our algorithm.

Learning an unknown Hamiltonian H from its dynamics $U(t) = e^{-iHt}$ is an important problem that arises in quantum sensing/metrology [1–9], quantum device engineering [10–15], and quantum many-body physics [16–23]. In quantum sensing/metrology, the Hamiltonian H encodes signals that we want to capture. A more efficient method to learn H implies the ability to extract these signals faster, which could lead to substantial improvement in many applications, such as microscopy, magnetic field sensors, and positioning systems. In quantum computing, learning the unknown Hamiltonian H is crucial for calibrating and engineering the quantum device to design quantum computers with lower error rates. In quantum many-body physics, the unknown Hamiltonian H characterizes the physical system of interest. Obtaining knowledge of H is hence crucial to understanding microscopic physics. A central goal in these applications is to find the most efficient approach for learning H .

In this work, we focus on the task of learning many-body Hamiltonians describing a quantum system with a large number of constituents. For concreteness, we consider an N -qubit system with geometrically-local interactions. Given any unknown N -qubit geometrically-local Hamiltonian H , we can represent H as

$$H = \sum_{a=1}^M \lambda_a E_a. \quad (1)$$

Here $\lambda_1, \dots, \lambda_M$ are the unknown parameters and $S = \{E_1, \dots, E_M\} \subseteq \{I, X, Y, Z\}^{\otimes N}$ is a subset of N -qubit Pauli operators. Each Pauli operator E_a acts nontrivially on at most $k = \mathcal{O}(1)$ qubits, and each qubit is acted on by $\mathcal{O}(1)$ of the Pauli operators in S . Many-body Hamiltonians with nearest-neighbor interactions on one-dimensional chains, two-dimensional square lattices,

three-dimensional cubic lattices are all special cases of geometrically-local Hamiltonians. The goal is to learn the parameters λ_a in the unknown Hamiltonian H . In previous works on learning many-body Hamiltonians [24–35], in order to reach an ϵ precision in estimating the parameters λ_a , the number of experiments and the total time required to evolve the system have a scaling of at least ϵ^{-2} . However, the ϵ^{-2} precision scaling is likely not the best-possible scaling for learning an unknown many-body Hamiltonian H .

In quantum sensing/metrology, the scaling of ϵ^{-2} for learning an unknown parameter to ϵ error is known as the standard quantum limit. For simple classes of Hamiltonians, such as a single-qubit Hamiltonian $H = \omega Z$ with unknown parameter ω , one can surpass the standard quantum limit using quantum-enhanced protocols [1, 3, 7, 36–38]. The true limit set by the basic principles of quantum mechanics is known as the Heisenberg limit, which suggests a scaling of ϵ^{-1} . There are two well-known approaches for achieving the Heisenberg limit for learning $H = \omega Z$. The first approach [3–5] considers evolving a highly-entangled state over $\ell = \mathcal{O}(\epsilon^{-1})$ qubits of the system under ℓ parallel Hamiltonian evolutions $(e^{-iHt})^{\otimes \ell}$ with $t = \mathcal{O}(1)$. The second approach [1, 39, 40] considers long-time coherent evolution $e^{-i\omega t Z}$ with $t = \mathcal{O}(\epsilon^{-1})$ over a single qubit. While the first approach was proposed earlier, the second approach has the advantage of requiring only a single qubit without entanglement.

The ϵ^{-1} scaling underlying the two approaches corresponds to the *total evolution time*. If a protocol uses J experiments, where the j -th experiment uses the unknown Hamiltonian evolution $e^{-iHt_{j,1}}, \dots, e^{-iHt_{j,K_j}}$, then the total evolution time is defined as

$$T \triangleq \sum_{j=1}^J \sum_{k=1}^{K_j} t_{j,k}. \quad (2)$$

In the first approach, each experiment uses $\mathcal{O}(\epsilon^{-1})$ constant time Hamiltonian evolutions in parallel, while the

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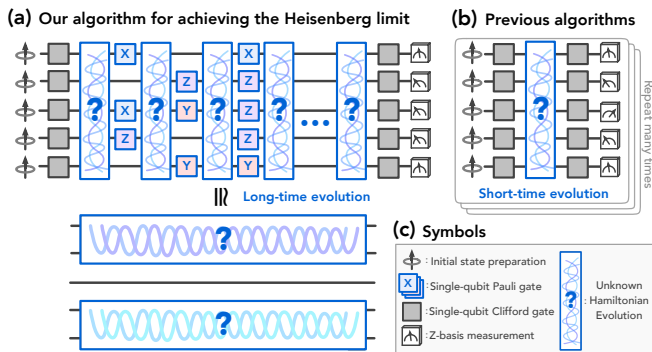


Figure 1. Algorithms for learning many-body Hamiltonians. (a) *Our algorithm for achieving the Heisenberg limit* ϵ^{-1} : We perform long-time coherent evolutions interleaved with random Pauli operators. The effective Hamiltonian is decoupled into non-interacting patches and can be efficiently learned. The algorithm only needs $\mathcal{O}(\text{polylog}(\epsilon^{-1}))$ experiments and a total evolution time of $\mathcal{O}(\epsilon^{-1})$. (b) *Previous algorithms for achieving the standard quantum limit* ϵ^{-2} : Previous methods [26, 29, 33, 34] repeatedly run a short-time evolution for many times. One needs $\mathcal{O}(\epsilon^{-2})$ experiments and a total evolution time of $\mathcal{O}(\epsilon^{-2})$. (c) *Symbols*: The symbols used in (a, b). The unknown Hamiltonian evolution is $U(t) = e^{-iHt}$.

second approach uses $\mathcal{O}(\epsilon^{-1})$ constant time Hamiltonian evolutions sequentially resulting in a single long time evolution. Both quantum sensing approaches result in a total evolution time of $\mathcal{O}(\epsilon^{-1})$.

These quantum-enhanced approaches could be applied to non-interacting systems as studied in multi-parameter quantum sensing [41–44]. However, they are challenging to apply in interacting systems with a large system size N and many unknown parameters. The difficulty stems from the many-body interactions in the Hamiltonian H . As time t becomes larger, the entanglement growth in e^{-itH} will cause all the unknown parameters in H to tangle with one another. The many-body entanglement can be seen as a form of decoherence, which kills the quantum enhancement. To prevent the system from becoming too entangled, prior work on learning many-body Hamiltonians focuses on a short time t , which loses the quantum enhancement and obtains, at best, an ϵ^{-2} scaling.

In this paper, we propose the first learning algorithm to achieve the Heisenberg limit for learning interacting many-body Hamiltonian. Figure 1 illustrates our algorithm. We prove the following performance guarantee.

Theorem 1. *There is an algorithm robust to state preparation and measurement (SPAM) error [45] that achieves the following: For any unknown N -qubit geometrically-local Hamiltonian $H = \sum_{a=1}^M \lambda_a E_a$ with $|\lambda_a| \leq 1$, after a total evolution time $T = \mathcal{O}(\epsilon^{-1} \log(\delta^{-1}))$, the learning algorithm can obtain estimates $\hat{\lambda}_a$ from the experiments, such that $\Pr \left[\left| \hat{\lambda}_a - \lambda_a \right| \leq \epsilon \right] \geq 1 - \delta$ for all $a \in \{1, \dots, M\}$.*

In quantum sensing and metrology, one often considers

the standard deviation of the estimate. We can show that to ensure the standard deviation $\sqrt{\mathbb{E}[\hat{\lambda}_a - \lambda_a]^2} \leq \epsilon$, we only need a total evolution time of $T = \mathcal{O}(\epsilon^{-1})$. This is because each estimate $\hat{\lambda}_a$ comes from a linear combination of $\mathcal{O}(1)$ eigenvalue estimates through a Hadamard transform, as shown in [46, Eq. (25)]. Each eigenvalue estimate has standard deviation at most $\mathcal{O}(\epsilon)$ as guaranteed by [40, Theorem I.1]. Consequently, their linear combination $\hat{\lambda}_a$ also has a standard deviation that scales as $\mathcal{O}(\epsilon)$. Hence, our algorithm saturates the Heisenberg limit in terms of the standard deviation. Our algorithm has the additional advantage of not requiring eigenstates or thermal states of the Hamiltonian H . Each of our experiments consists of the preparation of a noisy all-zero state $|0^N\rangle$, the evolution under the Hamiltonian H interleaved with single-qubit Clifford gates, and a noisy Z-basis measurement. The total number of experiments is only $\mathcal{O}(\text{polylog}(\epsilon^{-1}))$, which is significantly smaller than $\Theta(\epsilon^{-1})$. After running the experiments, the classical computational time to estimate all parameters is only $\mathcal{O}(N \text{polylog}(\epsilon^{-1}))$. Detailed statements can be found in [46, Theorems 13 and 21]. We note that our result generalizes to all low-intersection Hamiltonians as given in [46, Definition 2].

To establish the optimality of the proposed algorithm, we prove a matching lower bound.

Theorem 2. *Suppose there is a learning algorithm robust to SPAM error that achieves the following. For any unknown N -qubit geometrically-local Hamiltonian $H = \sum_{a=1}^M \lambda_a E_a$ with $|\lambda_a| \leq 1$, after a total evolution time T , the learning algorithm can obtain estimates $\hat{\lambda}_a$ from the experiments, such that $\Pr \left[\left| \hat{\lambda}_a - \lambda_a \right| \leq \epsilon \right] \geq 1 - \delta$ for all $a \in \{1, \dots, M\}$. Then, $T = \Omega(\epsilon^{-1} \log(\delta^{-1}))$.*

Thus, there is no algorithm that can perform asymptotically better than the one given in Theorem 1. Moreover, the lower bound can be seen as an algorithmic proof of the Heisenberg limit with the failure probability δ taken into account. It holds not only for algorithms with a fixed set of experiments but also for adaptive experiments that use information from previous experiment outcomes, following the set-up in [47–50].

In the following, we provide the ideas for designing the proposed learning algorithm and establishing the proof of the main results. All parts except for the last are devoted to Theorem 1. The last part is Theorem 2.

Reshaping an unknown Hamiltonian: A key technique used throughout the design of our learning algorithm is the idea of reshaping an unknown Hamiltonian using Hamiltonian simulation techniques. Recall that given a set of Hamiltonians H_1, \dots, H_K and the ability to implement the unitaries $e^{-itH_1}, \dots, e^{-itH_K}$, many Hamiltonian simulation techniques allow one to approximately implement the unitary $e^{-it \sum_{k=1}^K H_k}$. Note that these approximation formulas are valid for unitaries and no knowledge of the underlying Hamiltonian is required. As

such, they are applicable to the learning problem considered here.

For example, a randomized Hamiltonian simulation algorithm known as qDRIFT [51–53] considers an approximation (as a quantum channel) given by

$$e^{-it \sum_{k=1}^K H_k} \approx e^{-i(t/r)H_{k_r}} \dots e^{-i(t/r)H_{k_1}}, \quad (3)$$

where r is an integer that sets the approximation error, k_1, \dots, k_r are independent random variables sampled according to some probability distribution over $\{1, \dots, K\}$. Alternatively, we can also use the second-order Trotterization method [54–56] in our algorithm to reduce the asymptotic scaling of the number of Clifford gates required. Higher-order Trotterizations are not used because they require evolving backward in time.

Now, consider the unknown N -qubit Hamiltonian H which we hope to learn. We want to reshape it into the following Hamiltonian to facilitate learning:

$$\tilde{H} \triangleq \sum_{k=1}^K w_k H_k, \quad (4)$$

where $H_k \triangleq w_k U_k H U_k^\dagger$ and U_k is a unitary for each $k = 1, 2, \dots, K$. The weights $w_k \geq 0$. Any choice of unitaries U_k and weights w_k can be used. Later, to achieve the Heisenberg limit, we will choose specific U_k and w_k to ensure \tilde{H} disentangles the many-body system into noninteracting patches involving few qubits and has known eigenvectors irrespective of what H is. Our choice for each U_k will be a tensor product of Pauli operators. Using either qDRIFT or Trotterization, we only need to implement e^{-iH_k} , which can be done through $e^{-iH_k t} = U_k e^{-i(w_k t)H} U_k^\dagger$. To be more specific, we can implement $e^{-iH_k t}$ by first applying the unitary U_k^\dagger , letting the system evolve for time $w_k t$, and then applying U_k . Using Hamiltonian simulation techniques, we can evolve under the N -qubit unitary $e^{-it\tilde{H}}$. This reshaping technique is related to experimental approaches for engineering Hamiltonians through pulse sequences or strong fields [57–63]. Similar ideas have also been used to project H into the quantum Zeno subspace [64, 65]. The reshaping will lead to a small approximation error, which we discuss later (for a detailed discussion, see [46, Sections IV and VI]).

Learning a few-qubit Hamiltonian. We now show how the Hamiltonian reshaping technique is useful in learning Hamiltonians. We begin with a simple question: how to learn a few-qubit Hamiltonian on $\mathcal{O}(1)$ qubits with Heisenberg-limited precision scaling? If we naively apply quantum process tomography [49, 66–72] to learn the unknown Hamiltonian, we would have an ϵ^{-2} dependence in the number of measurements needed, where ϵ is the desired precision of the Hamiltonian parameters. Current methods with a Heisenberg-limited scaling typically require the Hamiltonian to be of a simple form, e.g., $H = \lambda X$ [1–9, 39, 40]. Therefore we need to consider a different method.

We show that for a few-qubit Hamiltonian, we can learn all the parameters involved using $\mathcal{O}(\epsilon^{-1} \log(\delta^{-1}))$ total evolution time, and $\mathcal{O}(\text{polylog}(\epsilon^{-1}) \log(\delta^{-1}))$ number of experiments. As an example, let us consider an arbitrary two-qubit Hamiltonian

$$H = \sum_{P, P' \in \{I, X, Y, Z\}} \lambda_{PP'} P \otimes P' \quad (5)$$

with $|\lambda_{PP'}| \leq 1$. Suppose we want to estimate the parameter λ_{XZ} . Then we can consider reshaping the unknown Hamiltonian H using $U_1 = I, U_2 = X_1, U_3 = Z_2, U_4 = X_1 Z_2$ and $w_1 = w_2 = w_3 = w_4 = \frac{1}{4}$. The new unknown Hamiltonian, after reshaping, is given by

$$\begin{aligned} \tilde{H} &\triangleq \frac{1}{4} (H + X_1 H X_1 + Z_2 H Z_2 + X_1 Z_2 H X_1 Z_2) \\ &= \lambda_{XZ} X_1 Z_2 + \lambda_{XI} X_1 + \lambda_{IZ} Z_2. \end{aligned} \quad (6)$$

The second equality is because the linear combination over the four terms eliminates all Pauli terms in H that do not have I or X on the first qubit and I or Z on the second qubit.

This new unknown Hamiltonian \tilde{H} gives us one crucial advantage: we have access to its eigenstates. This is because in \tilde{H} , for each qubit, there is only one (non-identity) Pauli operator associated with it. The eigenbasis for the new unknown Hamiltonian \tilde{H} is always given by $\{|+\rangle|0\rangle, |+\rangle|1\rangle, |-\rangle|0\rangle, |-\rangle|1\rangle\}$ regardless of the values of the unknown coefficients. We can use this information, together with the robust phase estimation algorithm in [40], to estimate the differences between pairs of eigenvalues, which in turn yield the parameters $\lambda_{XZ}, \lambda_{XI}, \lambda_{IZ}$ through a Hadamard transform. The procedure for applying random Pauli operators and obtaining parameters from eigenvalue estimation are described in detail in [46, Sections II.B and III.B]. By using different choices of U_1, \dots, U_4 to reshape H , we can get all the parameters $\lambda_{PP'}$ in the two-qubit Hamiltonian H . The same idea generalizes to arbitrary Hamiltonians on $\mathcal{O}(1)$ qubits.

Learning a many-qubit Hamiltonian through divide and conquer. If we want to learn a many-qubit Hamiltonian by directly applying the above method, the total evolution time will scale exponentially with the number of qubits. Here, we present a divide-and-conquer approach to address this problem. To illustrate the proposed approach, let us consider a simple example of an inhomogeneous Heisenberg model on N qubit with a Hamiltonian given by,

$$H = \sum_{\alpha=1}^{N-1} (\lambda_x^\alpha X_\alpha X_{\alpha+1} + \lambda_y^\alpha Y_\alpha Y_{\alpha+1} + \lambda_z^\alpha Z_\alpha Z_{\alpha+1}) \quad (7)$$

where $\lambda_x^\alpha, \lambda_y^\alpha, \lambda_z^\alpha$ are the unknown parameters, and $X_\alpha, Y_\alpha, Z_\alpha$ are the Pauli operators acting on qubit α . Suppose we want to learn the parameter λ_x^1 on the first two qubits. In order to achieve this, we reshape the unknown Hamiltonian H with $U_1 = I, U_2 = X_3, U_3 =$

$Y_3, U_4 = Z_3$ and $w_1 = w_2 = w_3 = w_4 = \frac{1}{4}$. The new unknown Hamiltonian after the reshaping is given by

$$\begin{aligned}\tilde{H} &= \frac{1}{4}(H + X_3HX_3 + Y_3HY_3 + Z_3HZ_3) \\ &= \tilde{H}_{1,2} + \tilde{H}_{\geq 4},\end{aligned}\quad (8)$$

where

$$\tilde{H}_{1,2} = \lambda_x^{1,2}X_1X_2 + \lambda_x^{1,2}Y_1Y_2 + \lambda_x^{1,2}Z_1Z_2, \quad (9)$$

and $\tilde{H}_{\geq 4}$ only contains terms acting on qubits $4, 5, \dots, N$. The second equality in (8) holds for the following reason: For each Pauli operator $P \in \{I, X, Y, Z\}^{\otimes N}$, if it acts non-trivially on the third qubit, then we can show that

$$\frac{1}{4}(P + X_3PX_3 + Y_3PY_3 + Z_3PZ_3) = 0. \quad (10)$$

On the other hand, for Pauli operator P that acts as identity on the third qubit, we can show that

$$\frac{1}{4}(P + X_3PX_3 + Y_3PY_3 + Z_3PZ_3) = P. \quad (11)$$

Therefore from (8), after the reshaping, the new Hamiltonian \tilde{H} does not generate entanglement between qubits 1, 2 and the rest of the system, and these two qubits evolve under the Hamiltonian $\tilde{H}_{1,2}$. This enables us to apply the learning algorithm for few-qubit Hamiltonians to $\tilde{H}_{1,2}$ to estimate λ_x^1 .

We can apply the above idea to learn every parameter in the Hamiltonian with a number of experiments that scales linearly in the system size N rather than exponential in N . We show that one could do better than linear scaling by a parallelization technique. In particular, we discuss how one could learn all the parameters $\lambda_x^1, \lambda_x^4, \lambda_x^7, \dots$ in parallel. Consider reshaping the unknown N -qubit Hamiltonian H given in Eq. (7) using $U_1 = I, U_2 = X_3X_6X_9 \dots, U_3 = Y_3Y_6Y_9 \dots, U_4 = Z_3Z_6Z_9 \dots$, and $w_1 = w_2 = w_3 = w_4 = 1/4$. Then the new Hamiltonian under reshaping is given by $\tilde{H} = \tilde{H}_{1,2} + \tilde{H}_{4,5} + \tilde{H}_{7,8} + \dots$, where $\tilde{H}_{\alpha, \alpha+1}$ is supported on qubits α and $\alpha+1$ for all $\alpha = 1, 4, 7, \dots$. Using a reshaping based on four unitaries U_1, \dots, U_4 , we have turned the unknown N -qubit interacting Hamiltonian H into a new Hamiltonian \tilde{H} with many noninteracting patches of two qubits. Each two-qubit patch is now evolving independently from each others. This decoupling enables us to estimate the parameters in parallel using the algorithm for learning few-qubit Hamiltonians.

This divide-and-conquer method works for any local Hamiltonian defined in (1). For this more general class of Hamiltonians, we determine how the reshaping is done by performing a coloring over its cluster interaction graph (a graph consisting of clusters of qubits that are acted on by a Pauli term in the Hamiltonian) [46, Lemma 5]. The coloring enables us to choose qubits, on which we apply

random I, X, Y, Z operators to decouple clusters of the same color from each other, thus enabling parallel estimation of the parameters associated with these clusters. For details, see [46, Sections I.B, II, and V]. A complete description of our algorithm for general local Hamiltonians can be found in [46, Algorithm 2]. The cost of the algorithm is summarized in [46, Theorem 13 and 21] (for the randomization and Trotterization approaches, respectively).

Characterizing approximation error in reshaping Hamiltonians. The estimation error of the proposed learning algorithm depends on the quantum measurement error as well as the approximation error when we reshape the unknown Hamiltonian into other forms. One way to analyze the approximation error is through the error analysis considered in [51] if we use qDRIFT to reshape or in [73] when using the second-order Trotter formula. However, these analyses are concerned with the error in the worst-case scenario over all possible input states and all observables. For the learning task given here, it leads to an overestimation of the approximation error as some key properties of the problem are not incorporated.

Consider the example of learning an inhomogeneous Heisenberg model on N qubits given in the previous section. To evolve under the N -qubit Hamiltonian reshaped \tilde{H} for time t , the analysis in [51] shows that the approximation error of qDRIFT with r steps is given by $\mathcal{O}(N^2t^2/r)$. Here, \tilde{H} is decoupled into many two-qubit patches that do not interact with each other, which prevents errors from propagating across the entire N -qubit system. We are interested only in the accuracy of evolving each patch, and the error from elsewhere in the system should not affect estimations of local observables. Similar considerations have been used to improve the error analysis of Hamiltonian simulation methods based on observable and initial state information [74–78]. In our case, a tighter analysis [79] using these facts shows that the approximation error is given by $\mathcal{O}(t^2/r)$ without an N dependence. We give the improved analysis for reshaping Hamiltonians using the randomization approach in [46, Section IV]. The improved analysis for using the second-order Trotter formula is given in [46, Section VI].

Establishing a matching lower bound. We prove a matching lower bound of $T = \Omega(\epsilon^{-1} \log(\delta^{-1}))$ on the total evolution time T [80]. The optimality with respect to the ϵ dependence is obtained by the Heisenberg limit. However, the optimality with respect to the failure probability δ has not been proven in the literature. We consider any learning algorithm that can run new experiments based adaptively on the outcomes of previous experiments. In order to handle adaptivity, we consider the rooted tree representation of the learning algorithm [48, 50], and consider the task of distinguishing between two distinct Hamiltonians $H_{\pm} = \pm \epsilon Z$.

We begin by considering how well one could use a single experiment to distinguish H_{\pm} , which is characterized by the total variation (TV) distance between the proba-

bility distribution over experimental outcomes under H_{\pm} . We characterize the TV distance in a single experiment. Then we consider an induction over every subtree of the learning algorithm to establish the TV distance over multiple experiments. A central technique is to control how each additional experiment improves one's ability to distinguish H_{\pm} . The proof of the lower bound is given in [46, Section VII].

Discussion. Our work shows that the Heisenberg limit can be achieved in the task of learning a large class of many-body local Hamiltonians with many unknown parameters. On the theoretical side, the central open question is whether our result can be extended to learning other classes of many-body Hamiltonians. For example, in an N -qubit Hamiltonian with all-to-all two-body interactions, our techniques achieve the Heisenberg limit with a quadratic dependence on system size N by learning all pairwise interactions one by one. This gives rise to the following question: can we achieve a scaling of $T = \mathcal{O}(\epsilon^{-1} \log(\delta^{-1}))$ for N -qubit Hamiltonians with all-to-all interactions? In addition to the above example, can we achieve the Heisenberg limit for learning fermionic or bosonic many-body Hamiltonians? Answering this question is important for applications such as reconstructing the structure of large molecules or learning the interactions in an exotic quantum material. Even more ambitiously, can one achieve the above scaling for learning the unknown parameters in an arbitrary N -qubit Hamil-

tonian without any structure? On the practical side, the central question is how to achieve the Heisenberg limit with minimal controllable quantum operations. For example, could one achieve the scaling $T = \mathcal{O}(\epsilon^{-1} \log(\delta^{-1}))$ for learning N -qubit local Hamiltonian H in a restricted model where we cannot interleave the unknown Hamiltonian evolution with single-qubit gates, and can only control state preparation and measurement? Understanding these questions will be crucial for physically achieving the Heisenberg limit in learning many-body Hamiltonians.

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