Quantum Algorithms for Testing Hamiltonian Symmetry

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Symmetries in a Hamiltonian play an important role in quantum physics because they correspond directly with conserved quantities of the related system. In this Letter, we propose quantum algorithms capable of testing whether a Hamiltonian exhibits symmetry with respect to a group. We demonstrate that familiar expressions of Hamiltonian symmetry in quantum mechanics correspond directly with the acceptance probabilities of our algorithms. We execute one of our symmetry-testing algorithms on existing quantum computers for simple examples of both symmetric and asymmetric cases.

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Introduction.—Symmetry is a key facet of nature that plays a fundamental role in physics [1,2]. Noether's theorem states that symmetries in Hamiltonians correspond with conserved quantities in the related physical systems [3]. The symmetries of a Hamiltonian indicate the presence of superselection rules [4,5]. In quantum computing and information, symmetry can indicate the presence of resources or lack thereof [6], and it can be useful for improving the performance of variational quantum algorithms [7–10]. Identification of symmetries can simplify calculations by eliminating degrees of freedom associated with conserved quantities—this is at the heart of Noether's theorem. This makes symmetries extraordinarily useful in the context of physics.

Quantum computing is a significantly younger field of study. First introduced as a quantum-mechanical model of a Turing machine [11], the intrigue of quantum computers lies in their potential to outperform their classical counterparts. The most obvious asset of quantum computers is the inherent physics behind the calculation, which includes nonclassical features such as superposition and entanglement. Classical simulations of quantum systems quickly become intractable as the size of the Hilbert space grows, needing exponentially many bits to explore the state space which multiple qubits naturally occupy. Intuitively, the quantum mechanical nature of these computers allows for simulations of quantum systems in a forthright way (see Ref. [12] and references therein).

A pertinent example of this, Hamiltonian simulation [13], garners high interest in the field [14–17]. Much work has been done toward understanding how to simulate these dynamics on quantum hardware such that they can be efficiently realized; however, to the best of our knowledge, there is currently no algorithm that tests Hamiltonian symmetries on a quantum computer, even though simulating Hamiltonians in this manner and identifying the symmetries of said Hamiltonians are both deemed to be of utmost importance.

In this Letter, we give quantum algorithms to test whether a Hamiltonian evolution is symmetric with respect to the action of a discrete, finite group. This property is often referred to as the covariance [18] of the evolution. If the evolution is symmetric, then the Hamiltonian itself is also symmetric, and thus, our algorithms test for Hamiltonian symmetry. Furthermore, we show that, for a Hamiltonian with an efficiently realizable unitary evolution, we can perform our first test efficiently on a quantum computer [17]. Here, "efficiently" means that the time necessary to complete the calculation to within a constant error bound scales, at most, polynomially with the number of qubits in the system. Our second quantum algorithm for testing Hamiltonian symmetry can be implemented by means of a variational approach [19,20]. The acceptance probabilities of both algorithms can be elegantly expressed in terms of familiar expressions of Hamiltonian symmetry [see Eqs. (13), (18), and (19)]. Here, we note that our algorithms can be understood as particular kinds of property tests [21] of quantum systems. As examples, we consider the transverse-field Ising model, the Heisenberg XY model [22], and the weakly J-coupled NMR Hamiltonian [23], whose evolution we test for various symmetry cases.

The consequences of such results extend throughout many areas of physics. Any study of a physical Hamiltonian can benefit from finding its symmetries, and our algorithms allow for an efficient check for these symmetries. With this knowledge, dynamics can be simplified by excluding symmetry-breaking transitions, calculations can be reduced into fewer dimensions, and intuition can be gained about the system of interest. Our first algorithm also scales well, meaning that systems too large and cumbersome to be studied by hand or classical computation can be investigated in a practical time scale, instead. Our quantum tests offer meaningful insight into physical dynamics.

In what follows, we begin by describing covariance symmetry of a unitary quantum channel—of which Hamiltonian dynamics are a special case. Next, we briefly review how Hamiltonian dynamics can be simulated on a quantum computer through the Trotter-Suzuki approximation [24]. Then, we present our main result—quantum algorithms to test the covariance symmetry of Hamiltonian dynamics. Finally, we demonstrate examples of symmetry tests on currently available quantum computers, and we discuss additional implications of our Letter.

Covariance of a quantum channel.—Before describing the symmetries of a Hamiltonian, first, we address the notion of covariance symmetry of a quantum channel [25]. Quantum channels transform one quantum state to another and are described by completely positive, trace-preserving maps. They serve as a convenient mathematical description of the dynamics induced by a Hamiltonian. The symmetries of a Hamiltonian naturally correspond to a covariance symmetry in the channel given by its evolution, and we exploit this in our algorithms.

We recall the established concept of covariance symmetry in more detail in Appendix A of the Supplemental Material [26], but briefly summarize the notion here. Suppose there is a channel sending Alice's quantum system to Bob's. For simplicity, we consider their systems to have the same dimension, though this is not required, in general. Further, suppose that we wish to determine whether this channel is symmetric with respect to some finite, discrete group G, which has a projective unitary representation [usually denoted $\{U(g)\}_{g\in G}$]. Then the channel is covariant if Alice, acting with her representation $U(g)$ before sending the system through the channel, is completely equivalent to Bob acting on his system with his representation of g after the state has been sent through the channel. In this sense, the channel commutes with the action of the group.

One method for testing this property given some channel involves using its Choi state, formally defined in Appendix A of [26]. The Choi state is generated by sending one half of a maximally entangled state through the channel, which, now, we assume to be unitary. Given the same group and its unitary representation, we define a projector

$$\Pi^G \coloneqq \frac{1}{|G|}\sum_{g\in G}\bar{U}_R(g)\otimes U_B(g), \tag{1}$$

onto the space of states of a composite system RB that are symmetric with respect to the group G, where the overline denotes complex conjugation. (Here, we use R to refer to a reference system and B to refer to Bob's system after the channel, a notion we use throughout.) The Choi state of the channel is equal to its projection onto the symmetric space if and only if the Choi state is symmetric with respect to G, given unitary representations of the system. If the Choi state of a channel exhibits this symmetry, then the channel itself is covariant [18], and the converse is true as well. This symmetry is necessarily dependent on the unitary representations used, although this is typically suppressed when referenced in the literature. We will also suppress this on the assumption that all representations are faithful.

This last notion of symmetry allows us to directly prescribe an algorithm to test for Hamiltonian symmetries. If we can emulate the dynamics of a Hamiltonian efficiently, we can test for the symmetry of its Choi state. The symmetry of the Choi state, then, directly implies symmetry of the Hamiltonian being tested.

Quantum simulations of Hamiltonians.—Quantum simulations provide a method for implementing Hamiltonian dynamics on quantum computers, usually by approximating them as sequences of quantum logic gates [12,13]. Much work has been conducted in this field, including work on implementations on near-term hardware [17,29], simulation by qubitization [30], simulation of operator spread [31], and more. Here, we review an example implementation.

One common approach [13] employs the Trotter-Suzuki approximation [24,32]. This method allows for decomposition into local Hamiltonian evolutions with some specified error. In this approximation, we suppose that the Hamiltonian H is of the form $H=\sum_{i=1}^{m}H_i$, where each H_i is a local Hamiltonian. Then, we can describe its evolution by

$$e^{-iHt}=\left(\prod_{j=1}^{m}e^{-iH_jt/r}\right)^r+\mathcal{O}\left(\frac{m^2t^2}{r^2}\right), \tag{2}$$

where the correction term is negligible for $mt/r\ll 1$ and vanishes when the terms in the decomposition commute (Here and throughout, we take $\hbar=1$). By other methods, the error can be reduced to higher orders in t [33].

An efficient quantum algorithm to test Hamiltonian symmetries.—Given the notion of covariance recalled above and a way to simulate the applicable Hamiltonian, now, we propose a quantum algorithm to test a Hamiltonian for covariance symmetry. We begin by supposing that we have a Hamiltonian composed of a finite sum of k local Hamiltonians, as described previously, with dynamics realized by higher-order methods such that the simulation error is $\mathcal{O}(t^4)$. Then, we claim a test for symmetries of this Hamiltonian with respect to a group G with a projective unitary representation $\{U(g)\}_{g\in G}$ can be performed efficiently on a quantum computer.

The circuit presented in Fig. 1 implements such a test, and we sketch its action here. Let the input state to the circuit be the maximally entangled state Φ_{RA}. Then, act on the A subsystem with the unitary Hamiltonian dynamics. As indicated in Fig. 1, the depth of the circuit to realize this algorithm can be cut in half by taking advantage of the

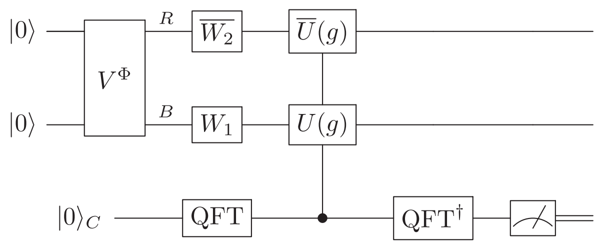

FIG. 1. Quantum circuit to test for the covariance of a unitary Hamiltonian evolution. The unitary V^{Φ} generates the state $|\Phi\rangle_{RA}$, the maximally entangled state on RA. The evolution of the system is given by $e^{-iHt} = W_1 W_2^{\dagger}$, and the $U(g)$ gates are controlled on a superposition over all of the elements $g \in G$, as in (4).

transpose trick $(X \otimes I)|\Phi\rangle = (I \otimes X^T)|\Phi\rangle$ and the decomposition $e^{-iHt} = W_1 W_2^{\dagger}$, which is clearly possible for Hamiltonian simulations of the form in (2) or from [33]. The state of the system is now given by

$$\Phi^t_{RB} \coloneqq (\mathbb{I}_R \otimes e^{-iHt})\Phi_{RA}(\mathbb{I}_R \otimes e^{iHt}), \tag{3}$$

which is exactly the Choi state of the channel generated by e^{-iHt}. Then, we use the quantum Fourier transform (QFT) to generate a control register in the following superposed state:

$$|+\rangle_C \coloneqq \frac{1}{\sqrt{|G|}} \sum_{g \in G} |g\rangle. \tag{4}$$

Implementing the controlled $\bar{U}(g)$ and $U(g)$ gates using the above control register yields the state

$$\frac{1}{|G|} \sum_{g,g' \in G} [\bar{U}_R(g) \otimes U_B(g)](\Phi^t_{RB} \otimes |g\rangle\langle g'|_C) \times [\bar{U}^{\dagger}_R(g') \otimes U^{\dagger}_B(g')]. \tag{5}$$

Finally, we perform the measurement $\mathcal{M} = \{|+\rangle\langle+|_C, \mathbb{I} - |+\rangle\langle+|_C\}$ on the control register and accept if and only if the outcome $|+\rangle\langle+|_C$ is observed. With this condition, the acceptance probability is given by

$$P_{\text{acc}} = \mathrm{Tr}[\Pi^G \Phi^t_{RB}], \tag{6}$$

where we have used the projector defined in (1) [see Appendix C of [26] for a quick derivation of (6)]. As a limiting case of the gentle measurement lemma [34–36], we have that

$$\mathrm{Tr}[\Pi^G \Phi^t_{RB}] = 1 \Leftrightarrow \Phi^t_{RB} = \Pi^G \Phi^t_{RB} \Pi^G, \tag{7}$$

where the second statement is equivalent to the condition on the Choi state given in Appendix A of [26]. Therefore, by implementing this algorithm, we can determine whether a Hamiltonian exhibits a symmetry under a group G with some projective unitary representation $\{U(g)\}_{g\in G}$. See Appendix B of [26] for further details of an approximate version of the equivalence in (7), which demonstrates that the acceptance probability is near to one if and only if the Choi state is approximately Bose symmetric.

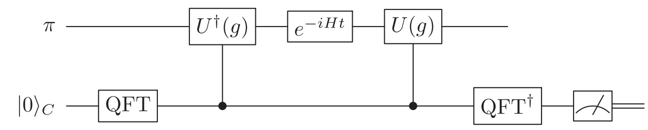

FIG. 2. Quantum circuit to test for the covariance of a unitary Hamiltonian evolution. Here, π denotes the maximally mixed state $\mathbb{I}/d$.

This algorithm can be further simplified. By invoking the transpose trick (see, e.g., Ref. [37]), we can identify the unitary on the reference system, $\bar{U}_R(g)$, with an equivalent action on A given by $U^{\dagger}_A(g)$. Since the action of the circuit would then take place solely on the subsystem A, the reference system R is traced out. This is equivalent to preparing the maximally mixed state (denoted by π) on A, such that this variation of our algorithm bears some resemblance to a one-clean-qubit algorithm [38] (also known as a DQC1 algorithm), with the exception that it requires $\log_2 |G|$ clean qubits for the control register. This simplification is shown in Fig. 2. The acceptance probability of the simplification described above is given by

$$P_{\text{acc}} = \frac{1}{d|G|} \sum_{g \in G} \mathrm{Tr}[U^{\dagger}(g) e^{iHt} U(g) e^{-iHt}], \tag{8}$$

where d is the dimension of the system being tested. Appendix C of [26] gives a proof that the expression in (8) is equal to the acceptance probability of the circuit in Fig. 1.

The proposed circuit is limited in complexity only by the implementation of the Hamiltonian and unitary representation. Thus, our first quantum algorithm is efficiently realizable. Furthermore, we have shown that entanglement resources, usually necessary for characterizing the Choi operator of a quantum channel, are not necessary here. We also note that the statistics accumulated for the maximally mixed state can be equivalently found in a sampling manner using computational basis state inputs.

We note that the acceptance probability given in (8) bears some resemblance to a group-averaged out-of-time-order correlator (OTOC) [39–41], a measure of near-time quantum chaos. Previous work gave an efficient quantum algorithm for estimating an OTOC [42]; however, their work did not consider symmetry transformations of Hamiltonian evolutions nor have the group-symmetric structure considered here. Additionally, a continuous group-averaged OTOC was shown to relate to the spectral form factor [39], a measure of late-time chaos in a system. However, it is unclear how this quantity would be interpreted for a discrete group rather than a continuous group such as previously investigated.

To provide evidence that our algorithm cannot generally be simulated efficiently by classical computers, we turn to established notions of computational complexity. In Appendix D of [26], we prove that estimating the acceptance probability in (8) to within additive error is a DQC1-complete problem. This means that (8) can be estimated within this restricted model of quantum computing (via our algorithm and by an observation of [[43], Section 1]). Furthermore, this demonstrates that estimating (8) is just as computationally hard as any problem in this complexity class. Strong evidence exists that classical computers cannot solve DQC1-complete problems efficiently [44,45], thus, ruling out any possibility of estimating the acceptance probability in (8) by a classical sampling approach. See Appendix D of [26] for further details and discussions.

A derivation of symmetry in the acceptance probability.—From the acceptance probability given in (8), we can derive a relationship with the familiar expression of Hamiltonian symmetry in quantum mechanics, further establishing this as an authentic test of symmetry. Consider expanding e^{iHt}, under the assumption that $\tau \coloneqq \|H\|_\infty t < 1$, where $\|X\|_\infty \coloneqq \sup_{|\psi\rangle\neq 0}(\|X|\psi\rangle\|_2/\||\psi\rangle\|_2)$

$$e^{iHt} = \mathbb{I} + iHt - \frac{H^2t^2}{2} - \frac{iH^3t^3}{6} + \mathcal{O}(\tau^4). \tag{9}$$

Substituting this relation into the trace argument of (8), we find that

$$\begin{aligned}\mathrm{Tr}[U^\dagger e^{iHt} U e^{-iHt}] = d &+ t^2(\mathrm{Tr}[HU^\dagger HU] - \mathrm{Tr}[H^2]) \\ &+ \frac{it^3}{2}(\mathrm{Tr}[U^\dagger H^2 UH] - \mathrm{Tr}[U^\dagger HUH^2]) \\ &+ \mathcal{O}(\tau^4),\end{aligned} \tag{10}$$

where the equality is obtained using the linearity and cyclicity properties of the trace. After summing over all group elements, as in (8), and using the group property (that $g\in G$ implies $g^{-1}\in G$), we find that $(1/|G|)\times \sum_{g\in G}\{\mathrm{Tr}[U^\dagger(g)H^2U(g)H] - \mathrm{Tr}[U^\dagger(g)HU(g)H^2]\} = 0$, so that the third order term of (8) vanishes. We can simplify the second order term of (8) by using

$$\frac{1}{2}\mathrm{Tr}[|[U,H]|^2] = -\mathrm{Tr}[HU^\dagger HU] + \mathrm{Tr}[H^2], \tag{11}$$

where $|X|^2 \coloneqq X^\dagger X$ implies that

$$|[U,H]|^2 = H^2 - HU^\dagger HU - U^\dagger HUH + U^\dagger H^2 U. \tag{12}$$

Putting these equations together, we can rewrite the acceptance probability of our first quantum algorithm elegantly as

$$P_{\mathrm{acc}} = 1 - \frac{t^2}{2d|G|}\sum_{g\in G}\|[U(g),H]\|_2^2 + \mathcal{O}(\tau^4), \tag{13}$$

where $\|A\|_2 \coloneqq \sqrt{\mathrm{Tr}[|A|^2]}$ is the Hilbert-Schmidt norm. Thus, to the first nonvanishing order of time t, the acceptance probability is equal to one if and only if

$$[U(g),H] = 0, \quad \forall\ g\in G. \tag{14}$$

This is exactly the familiar expression for symmetry. Furthermore, the expression in (13) clarifies that the normalized commutator norm $(1/d|G|)\sum_{g\in G}\|[U(g),H]\|_2^2$ can be estimated efficiently by employing our algorithm. From (13), we can see that the normalized commutator norm is small—equivalently, the Hamiltonian H is approximately symmetric—if and only if the acceptance probability is close to one. (See [[46], Sections III and V] or [6] for further discussions on asymmetry fluctuations.) Finally, as we show in Appendix E of [26], the acceptance probability has an exact expansion as follows, such that all odd powers in t vanish, and the even powers are scaled by normalized nested commutator norms, quantifying higher orders of symmetry

$$P_{\mathrm{acc}} = \sum_{n=0}^{\infty}\frac{(-1)^n t^{2n}}{(2n!)}\left(\frac{1}{d|G|}\sum_{g\in G}\|[(H)^n, U(g)]\|_2^2\right), \tag{15}$$

where the nested commutator is defined as

$$[(X)^n, Y] \coloneqq \underbrace{[X,\cdots[X,[X}_{n\,\mathrm{times}},Y]]\cdots], \qquad [(X)^0,Y]\coloneqq Y. \tag{16}$$

Note that the expansion in (15) is valid for all $t\in\mathbb{R}$. We also provide an alternative formula for P_{acc} in Appendix E of [26].

Variational quantum algorithm for symmetry testing.—Rather than feeding in the maximally mixed state to the input of the circuit in Fig. 2, we can feed in an arbitrary input state $|\psi\rangle$, instead. As shown in Appendix F of [26], the acceptance probability when doing so is equal to

$$\|\mathcal{T}_G(e^{-iHt})|\psi\rangle\|_2^2 = 1 - t^2\langle\mathcal{T}_G(H^2) - [\mathcal{T}_G(H)]^2\rangle_\psi + O(\tau^3), \tag{17}$$

where $\mathcal{T}_G(X) \coloneqq (1/|G|)\sum_{g\in G}U(g)XU^\dagger(g)$. Note that the bracketed term is non-negative as a consequence of the Kadison-Schwarz inequality [[47], Theorem 2.3.2]. If we had the ability to prepare arbitrary quantum states (modeled in [48]), we could optimize this acceptance probability over all states, resulting in the following value:

$$\|\mathcal{T}_G(e^{-iHt})\|_\infty^2 \geq 1 - \frac{2}{|G|}\sum_{g\in G}\|[U(g), e^{-iHt}]\|_\infty \tag{18}$$

$$\geq 1 - \frac{2t}{|G|}\sum_{g\in G}\|[U(g),H]\|_\infty - 4\tau^2. \qquad (19)$$

These inequalities are proven in Appendix F of [26], and the second holds under the assumption that $\tau < 1$. This demonstrates that the acceptance probability $\|\mathcal{T}_G(e^{-iHt})\|_\infty^2$ can be bounded from below in terms of a familiar expression of Hamiltonian symmetry. Thus, if the commutator norm $(1/|G|)\sum_{g\in G}\|[U(g),H]\|_\infty$ is small, as is the case when the Hamiltonian is approximately symmetric, then the acceptance probability of this algorithm is close to one. In Appendix F of [26], we also prove that the acceptance probability satisfies

$$\|\mathcal{T}_G(e^{-iHt})\|_\infty^2 \geq \left(1 - \sum_{n=1}^{\infty}\frac{t^n}{n!}\frac{1}{|G|}\sum_{g\in G}\|[(H)^n, U(g)]\|_\infty\right)^2. \qquad (20)$$

Since it is physically impossible to optimize over all input states, instead, we can employ a variational ansatz to do so, in order to arrive at a lower bound estimate of the acceptance probability on the left-hand side of (18). These methods have been vigorously pursued in recent years in the quantum computing literature [19,20], and they can be combined with our approach here. In short, the acceptance probability in (17) is a reward function that can be estimated by means of the circuit in Fig. 2 and a parametrized circuit that prepares the state $|\psi\rangle$. Then, one can employ gradient ascent on a classical computer to modify the parameters used to prepare the state $|\psi\rangle$. After many iterations, these algorithms typically converge to a value, which, in our case, provides a lower bound estimate of the acceptance probability on the left-hand side of (18). In practice, it might be difficult in experiments to optimize over all pure states, and instead, one could consider a variational product state ansatz, as in [49].

Examples.—To exhibit our algorithm, we consider the dynamics given by the transverse Ising model (TIM) with a cyclic boundary condition. This Hamiltonian is given as $H_{\mathrm{TIM}} \coloneqq \sigma_N^Z \otimes \sigma_1^Z + \sum_{i=1}^{N-1}\sigma_i^Z \otimes \sigma_{i+1}^Z + \sum_{i=1}^{N}\sigma_i^X$. This Hamiltonian is permutationally invariant, so that $[H_{\mathrm{TIM}}, W^\pi] = 0$ for all $\pi \in S_N$, where W^π is a unitary representation of the permutation $\pi \in S_N$, with S_N denoting the symmetric group of N elements. It also obeys the symmetry $[H_{\mathrm{TIM}}, \sigma_1^X \otimes \cdots \otimes \sigma_N^X] = 0$. Thus, we can use our algorithm to test these symmetries, and we do so in Fig. 3 for $N = 3$ and $N = 4$. (Rather than test all permutations, here, we indicate that we test for invariance under a cyclic shift.) We find that each respective symmetry test passes with reasonable probability, with deviation from one due to noise added to the simulation. In Appendix G of [26], we implement symmetry tests for two other examples—the weakly J-coupled NMR Hamiltonian and the Heisenberg XY model. Here, we note that all computer

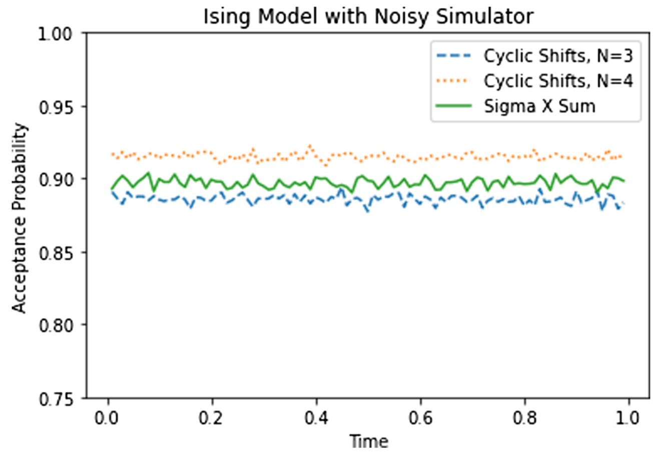

FIG. 3. Results of symmetry tests for the transverse Ising model for $N = 3$ and $N = 4$, using IBM Quantum's noisy simulator. The symmetries in question are given by acting simultaneously on all systems by either the cyclic group of order N or a conjugation by $(\sigma^X)^{\otimes N}$.

codes used to generate the examples in the main text and the Supplemental Material are available online [50].

Conclusion.—In this Letter, we have specified algorithms to test a Hamiltonian for symmetry with respect to a group. Our first test is efficiently realizable given similarly efficient Hamiltonian simulations, and our second test employs a variational approach. These algorithms are useful tools that we suspect should be of interest throughout many realms of physics.

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