Quantum Simulation of Time-Dependent Hamiltonians and the Convenient Illusion of Hilbert Space

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We consider the manifold of all quantum many-body states that can be generated by arbitrary time-dependent local Hamiltonians in a time that scales polynomially in the system size, and show that it occupies an exponentially small volume in Hilbert space. This implies that the overwhelming majority of states in Hilbert space are not physical as they can only be produced after an exponentially long time. We establish this fact by making use of a time-dependent generalization of the Suzuki-Trotter expansion, followed by a well-known counting argument. This also demonstrates that a computational model based on arbitrarily rapidly changing Hamiltonians is no more powerful than the standard quantum circuit model.

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The Hilbert space of a quantum system is big—its dimension grows exponentially with the number of particles it contains. Thus, parametrizing a generic quantum state of N particles requires an exponential number of real parameters. Fortunately, the states of many physical systems of interest appear to occupy a tiny submanifold of this gigantic space. Indeed, the essential physical features of many systems can be explained by variational states specified with a small number of parameters. Well-known examples include the BCS state for superconductivity [1], Laughlin's state for fractional quantum Hall liquids [2], and tensor network states occurring in real-space renormalization methods [3]. In these cases, the number of parameters scales only polynomially with N.

In this Letter, we attempt to define the class of *physical* states of a many-body quantum system with local Hilbert spaces of bounded dimensions and prove that they represent an exponentially small submanifold of the Hilbert space. We say that a state is physical if it can be reached, starting in some fiducial state (e.g., a ferromagnetic state, or the vacuum), by an evolution generated by any time-dependent quantum many-body Hamiltonian, with the constraint that (1) the Hamiltonian is local in the sense that it is the sum of terms each acting on at most k bodies for some constant k independent of N, and (2) the duration of the evolution scales at most as a polynomial in the number of particles in the system. The duration of the evolution has a meaning only if there is a well-defined time or energy scale. We do this by setting the strength of the local terms in the Hamiltonian to some constant E. Such bounded interaction strength is crucial to our derivation. The assumption about the initial fiducial state is artificial; we could alternatively define the class of physical evolutions for quantum many-body systems as the ones generated by Hamiltonians obeying constraints (1) and (2), and would reach the same conclusions.

The second constraint is very much reminiscent of the way complexity classes are defined in theoretical computer science, where the central object of study is the scaling of the time required to solve a problem as a function of its input size. The classical analogue for the problem that we address is a well-known counting argument of Shannon [4] demonstrating that the number of Boolean functions of N bits scales doubly exponentially (as 2^{2^N}), with the consequence that no efficient (i.e., polynomial) algorithm can exist to compute the overwhelming majority of those functions. Indeed, the number of different functions that can be encoded by all classical circuits of polynomial depth scale as $2^{\mathrm{poly}(N)}$, which is exponentially smaller than the total number of Boolean functions.

Our contribution is a quantum generalization of this result. The crux of our argument is to demonstrate that the dynamics generated by any local Hamiltonian, without any assumptions on its time dependence, can be simulated by a quantum circuit of polynomial size. All previously known simulation methods [5–10] produced a quantum circuit of complexity that depends on the smoothness of the Hamiltonian, scaling, e.g., with $\|\partial H/\partial t\|$ or some higher derivatives. Using the results of Huyghebaert and De Raedt [11], we show how these conditions can be overcome. We then use a well-known counting argument [12] for quantum circuits that involves the Solovay-Kitaev theorem [13] to arrive at the conclusion that most states in the Hilbert space are not physical: they can only be reached after an exponentially long time. Note that a direct parameter counting would not produce this result because we impose no restriction on the time dependence of the Hamiltonian. The complete description of a rapidly changing Hamiltonian requires lots of information, so

from this perspective there are in principle enough parameters to reach all states in the Hilbert space.

Our demonstration that arbitrary local time-dependent Hamiltonians can be efficiently simulated on quantum computers is of interest in its own right in the context of quantum computation. More precisely, we are concerned with Hamiltonians acting on N particles of the form

$$H(t) = \sum_{X \subset \{1,2,\ldots,N\}} H_X(t), \tag{1}$$

where X labels subsets of the N particles, each term has bounded norm $\|H_X(t)\| \leq E$, and each term acts on no more than k particles, i.e., $H_X(t) = 0$ if $|X| > k$, and k is fixed, independent of the system size. We make no assumption on the geometry of the system, and the coupling can be arbitrarily long ranged. The time-evolution operator $U(0, t)$ from time 0 to t is governed by Schrödinger's equation $\frac{d}{dt}U(0, t) = -iH(t)U(0, t)$, with solution given in terms of a time-ordered integral $U(0, t) = \mathcal{T} \exp\{\int_0^t H(s)ds\}$.

Starting with Feynman's exploration of quantum computers [14], it has been well established that the time-evolution operator generated by Hamiltonians of the form Eq. (1) can be decomposed into short quantum circuits, provided that $H(t)$ varies slowly enough [5–10]. In all cases, this is achieved by approximating the evolution operator by a *product formula*

$$U(0, t) \approx \prod_{p=1}^{N_P} \exp\{-iH_{X_p}(t_p)\Delta t_p\}, \tag{2}$$

where the sequences X_p, t_p, and Δt_p are set by specific approximation schemes, such as the Trotter formula [15] or the Lie-Suzuki-Trotter formula [16]. Because each term H_X acts on at most k particles, this last expression represents a sequence of k-body unitaries. A standard quantum circuit is obtained by simulating each of these k-body operators as a sequence of one- and two-qubit gates using the result of Solovay-Kitaev [13,17].

Perhaps the simplest example of a product formula decomposition of $U(0, t)$ is given by

$$U(0, t) \approx \prod_{j=1}^{n} \prod_{X} \exp\{-iH_X(j\Delta t)\Delta t\}, \tag{3}$$

where the product over X can be carried in any given order. This decomposition makes use of two approximations. First, the time dependence of the $H(t)$ is ignored on time scales lower than Δt: the Hamiltonian is approximated by a piecewise constant function taking the values $H(j\Delta t)$ on the time interval $[(j-1)\Delta t, j\Delta t]$. Second, each matrix exponential is decomposed using the Trotter formula $\exp\{-iH(t)\Delta t\} \approx \prod_X \exp\{-iH_X(t)\Delta t\}$. Clearly, the size Δt of the time intervals must be shorter than the fluctuation time scale of $H(t)$ for the first approximation to be valid, $\Delta t \ll \|\partial H/\partial t\|^{-1}$. Higher frequency fluctuations would therefore require breaking the time evolution into shorter intervals, thus increasing the overall complexity of the simulation.

Time-dependent Trotter-Suzuki expansion.—Somewhat surprisingly, it is possible to generalize the Trotter-Suzuki formula to time-dependent Hamiltonians without compromising the error, where the Hamiltonian may exhibit fluctuations much faster than the time step Δt. We begin by breaking the total time evolution into short segments $U(0, t) = U(t_n, t_n + \Delta t)\ldots U(t_2, t_2 + \Delta t)U(0, 0 + \Delta t)$, each of duration Δt

$$U(t_j, t_j + \Delta t) = \mathcal{T} \exp\left(-i \int_{t_j}^{t_j+\Delta t} ds \sum_X H_X(s)\right).$$

In the simple case where the sum over X contains only two terms, say H_1 and H_2, it has been shown [11] that the generalized Trotter-Suzuki expansion

$$U^{\mathrm{TS}}(t_j, t_j + \Delta t) = \mathcal{T} \exp\left(-i \int_{t_j}^{t_j+\Delta t} ds H_1(s)\right) \times \mathcal{T} \exp\left(-i \int_{t_j}^{t_j+\Delta t} ds H_2(s)\right)$$

gives an error in terms of the operator norm that is

$$\|U(t_j, t_j + \Delta t) - U^{\mathrm{TS}}(t_j, t_j + \Delta t)\| \leq c_{12}(\Delta t)^2,$$

with c_{12} of the order of 1 and given by

$$c_{12} = \frac{1}{(\Delta t)^2} \int_{t_j}^{t_j+\Delta t} dv \int_{t_j}^{v} du \|[H_1(u), H_2(v)]\|.$$

c_{12} is upper bounded by $c_{\max}^2/2$ with $c_{\max} = \max_X \|H_X\|$, with $\|H_X\| = \sup_{0 \leq s \leq t} \|H_X(s)\|$. Note that this bound does not depend on the derivative of the Hamiltonian (and is therefore also valid for nonanalytic time dependence). Note also that the bound reduces to the usual Trotter error for the time-independent case and is therefore equally strong, and that it can straightforwardly be generalized to higher order decompositions.

For our present application, the Hamiltonian is the sum of $L \in \mathrm{poly}(N)$ k-particle terms, cf. Eq. (1). We can therefore iterate the above procedure $\log_2(L)$ times; at the nth iteration, there are 2^n terms, each of strength upper bounded by $c_{\max}L/2^n$. The total error for approximating the exact time evolution of the Hamiltonian with L terms by a product of L time-ordered terms is

$$\frac{1}{2} c_{\max}^2 (\Delta t)^2 \sum_{m=1}^{\log_2 L} 2^m \left(\frac{L}{2^m}\right)^2 \leq \frac{1}{2} c_{\max}^2 L^2 (\Delta t)^2,$$

which can be made arbitrary small by choosing a Δt that scales as an inverse polynomial in N. Approximating the time-evolution operator over a total time t with a product of k-body unitaries, such that the total error is $\epsilon/2$, can therefore be achieved by choosing $\Delta t = \frac{\epsilon}{t c_{\max}^2 L^2}$. The total number G of k-body unitaries to achieve this accuracy is then equal to $G(\epsilon, L, t) = L \frac{t}{\Delta t} = \frac{c_{\max}^2}{\epsilon} t^2 L^3$.

The value of each such k-body unitary can be obtained by solving the corresponding finite time-ordered integral on a classical computer. The Solovay-Kitaev (SK) theorem [13,17] shows that each of these k-body unitary transformations can be simulated with standard one- and two-qubit gates chosen from a fixed discrete set (e.g., CNOT's between any pair of qubits supplemented by a local $\pi/8$ rotation gate). To achieve an accuracy ϵ_G per unitary transformation, we need $d_{\mathrm{SK}}[\log_2^{c_{\mathrm{SK}}}(1/\epsilon_G)]$ standard gates with c_{SK} and d_{SK} constants; we choose ϵ_G such that $\epsilon_G = \frac{\epsilon}{2G(\epsilon,L,t)}$. The total number of quantum gates as chosen from a discrete set of gates needed to approximate the complete time evolution with an error ϵ is therefore upper bounded by $G_{\mathrm{tot}}(\epsilon, L, t) = d_{\mathrm{SK}} G(\epsilon, L, t) \log_2^{c_{\mathrm{SK}}}[G(\epsilon, L, t)/\epsilon]$, which is polynomial in the number of qubits; it roughly scales quadratically in t and as the cube of the total number of (noncommuting) local terms in the Hamiltonian.

Average Hamiltonians and randomized evolution.—Note that the time-dependent Trotter-Suzuki decomposition described in the previous section does not lead to a product formula because each term appearing in it involves a time-ordered integral $U_X(t_j, t_j + \Delta t) = \mathcal{T} \exp\{-i \int_{t_j}^{t_j+\Delta t} H_X(s) ds\}$ rather than the exponential of a term of the Hamiltonian at a given time $\exp\{-i \Delta t H_X(t)\}$ as in Eq. (2). Although this does not affect the conclusions reached in the next section on the counting of possible quantum states, it is unsatisfactory from the point of quantum simulation. In this section, we demonstrate how to recover a product formula by making use of randomness. In Ref. [18], product formula decompositions Eq. (2) were found for any local Hamiltonian, where the number of terms N_P in the product depends on a smoothness parameter $\Lambda_P = \sup_{0 \le p \le P, 0 \le s \le t} \sum_X (\| \partial_s^p H_X(s) \|)^{1/(p+1)}$. In particular, these decompositions are inefficient when the fluctuation time scale of the Hamiltonian becomes too small. Our methods circumvent these requirements by using randomness. Further, randomization avoids the complexity of integration.

We do this in two steps. First, we replace the time-ordered exponential integral with the exponential of an ordinary integral without introducing a significant error. Indeed, we show in Appendix A in the supplemental material [19] that

$$\left\| \mathcal{T} \exp\left\{ -i \int_{t_j}^{t_j+\Delta t} ds H_X(s) \right\} - \exp\left\{ -i \int_{t_j}^{t_j+\Delta t} ds H_X(s) \right\} \right\| \le \frac{2}{3} \|H_X\|^2 \Delta t^2. \quad (4)$$

Using this result, we obtain the approximate decomposition

$$U(0, t) \approx \prod_{j=1}^{n} \prod_X \exp\left\{ -i \int_{t_j}^{t_j+\Delta t} H_X(s) ds \right\}.$$

Note that this is still *not* a product formula because it involves integrals. This first step has nevertheless eliminated the need of a time-order operator.

The second step to obtain a product formula for $U(0, t)$—one that does not require any integrals—makes use of randomness. The average Hamiltonian $H_{X,j}^{\mathrm{av}}$ on the interval $[(j-1)\Delta t, j\Delta t]$ can be estimated using Monte Carlo integration. For every j, we can pick m random times $\tau_j^k \in [t_j, t_j + \Delta t]$ and approximate $H_{X,j}^{\mathrm{av}} \approx \frac{1}{m} \sum_{k=1}^m H_X(\tau_j^k)$. Because the variance of the Hamiltonian is bounded by $\|H_X\|^2$, the sum converges to $H_{X,j}^{\mathrm{av}}$ with error estimate $\Delta t \|H_X\|/\sqrt{m}$. Using this Monte Carlo average, we can approximate the evolution operator of the time interval $[t_j, t_j + \Delta t]$ by

$$U_X^{\mathrm{av}}(t_j, t_j + \Delta t) \approx \exp\left\{ -i \frac{1}{m} \sum_{k=1}^{m} H_X(\tau_j^k) \right\} \quad (5)$$

$$\approx \prod_{k=1}^{m} \exp\left\{ -i \frac{\Delta t}{m} H_X(\tau_j^k) \right\}, \quad (6)$$

where the order of the product can be chosen according to increasing values of τ_j^k. The error in the first approximation Eq. (5) is set by the Monte Carlo estimate $\Delta t \|H_X\|/\sqrt{m}$ while the second approximation Eq. (6) is the usual Trotter-Suzuki formula. Summarizing, we can decompose the total evolution operator from time 0 to t as $U(0, t) \approx \prod_{j,k,X} \exp\{-i \frac{\Delta t}{m} H_X(\tau_j^k)\}$, where the product should be taken in increasing order of τ_j^k and any order of X. This is a standard product formula like Eq. (2)—identical to the usual decomposition explained in the introduction [Eq. (3)] and the one presented in [18]—except that the times τ_j^k at which the Hamiltonian is sampled are *random*. Thus, we see that by sampling the Hamiltonian at random times, we completely circumvent any smoothness requirements [20].

We note that the proof of Eq. (4) is an illustration of the *decoupling* principle that tells us that the high-frequency fluctuations of the Hamiltonian should not affect the low-energy physics. As a consequence, it is possible to largely ignore these fluctuations—by replacing the time-dependent Hamiltonian by its average value on each time bin—without significantly modifying the dynamics of the system. This is the working principle behind renormalization group methods of quantum field theory and quantum many-body physics. The rotating wave approximation [21] and effective Hamiltonian theory [22] are simple examples illustrating this principle in the case of time-dependent Hamiltonians.

More generally, we show in Appendix B of the supplemental material [19] that we can replace the time-dependent Hamiltonian $H(t)$ with a smoothed version $\tilde{H}(t)$ with fluctuation time scale bounded by σ without significantly affecting the resulting time-evolution operator. More precisely, we show that the time-evolution operators from time 0 to t differ by at most $\|H\|^2 t \sigma$.

Counting states.—Let us now consider the set of all quantum states that can be reached starting from some fiducial state $|0\rangle$ and evolving for some polynomial amount

of time under any time-dependent Hamiltonian. A direct counting argument appears difficult because there are infinitely many distinct time-dependent Hamiltonians, and therefore there can *a priori* be infinitely many states in that set. However, we just established that the time-evolution operator generated by any one of these Hamiltonians can be well approximated by a polynomial-size quantum circuit built from a fixed set of M discrete gates for some constant M.

Thus, to count the number of states that can be produced by arbitrary time-dependent Hamiltonians, it suffices to count the number of polynomial-size quantum circuits constructed from a universal discrete set of one- and two-qubit gates, and to consider an ε ball around the output of each of these circuits, i.e., the set of states within a distance ε of the outputs of these circuits. Surely, the states reached in polynomial time by arbitrary time-dependent Hamiltonians are contained in the union of these balls. It is well known [12] that such circuits can only reach exponentially small subset of states.

Since we limit the evolution to polynomial time, there exists a constant α such that the total number of gates in the simulation circuit is bounded by K^α, where $K \propto N$ is the number of qubits required for the simulation. There are no more than $N_{\text{circuits}} = (MK^2)^{K^\alpha}$ distinct ways of arranging these gates into a quantum circuit (M possibility for each gate and K^2 possible pairs of qubits between which it can be applied), and therefore no more than N_{circuits} distinct states that can be produced. On the other hand, the states of K qubits live on a $(2^{K+1}-1)$-dimensional hypersphere, whose surface area is $S = 2\pi^{2^K}/\Gamma(2^K)$, and an ε ball around a given state is a $(2^{K+1}-2)$-dimensional hypersphere of volume $V = 2\pi^{2^K-1}\varepsilon^{2^{K+1}-2}/\Gamma(2^K)$. Combining, we see that the ε balls of physical states occupy only an exponentially small fraction $\frac{N_{\text{circuits}}V}{S} = \mathcal{O}(K^K\epsilon^{2^K})$ of the total volume in Hilbert space. Thus, the overwhelming majority of states in the Hilbert space of a quantum many-body system can only be reached after a time scaling exponentially with the number of particles.

Conclusion—We demonstrated that any time-dependent local Hamiltonian can be simulated efficiently using a quantum computer, independent of the frequencies involved. As an application, we showed that the set of quantum states that can be reached from a product state with a polynomial-time evolution of an arbitrary time-dependent quantum Hamiltonian is an exponentially small fraction of the Hilbert space. This means that the vast majority of quantum states in a many-body system are unphysical, as they cannot be reached in any reasonable time. As a consequence, all physical states live on a tiny submanifold, and that manifold can easily be parametrized by all poly-sized quantum circuits. Although quantum circuits are unitary and do not directly simulate imaginary time evolution, the counting argument we presented holds equally well in this setting, and hence thermal and ground states of local Hamiltonians are also efficiently parametrized by short circuits. This raises the question of whether it makes sense to describe many-body quantum systems as vectors in a linear Hilbert space. The recent advances in real-space renormalization group methods [3,23,24] indeed seem to suggest that a viable approach consists of parametrizing quantum many-body states using tensor networks and quantum circuits.

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