Nonlocal Hamiltonian simulation assisted by local operations and classical communication

G. Vidal[1,2] and J. I. Cirac[1]
[1]*Institut für Theoretische Physik, Universität Innsbruck, A-6020 Innsbruck, Austria*
[2]*Institute for Quantum Information, California Institute of Technology, Pasadena, California 91125*
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Consider a set of N systems and an arbitrary interaction Hamiltonian H that couples them. We investigate the use of local operations and classical communication (LOCC), together with the Hamiltonian H, to simulate a unitary evolution of the N systems according to some other Hamiltonian H'. First, we show that the most general simulation using H and LOCC can also be achieved, with the same time efficiency, by just interspersing the evolution of H with local unitary manipulations (LU) of each system and a corresponding local ancilla (in a so-called LU+anc. protocol). Thus, the ability to make local measurements and to communicate classical information does not help in nonlocal Hamiltonian simulation. Second, we show that both for the case of two d-level systems ($d>2$), or for that of a setting with more than two systems ($N>2$), LU+anc. protocols are more powerful than LU protocols. Therefore local ancillas are a useful resource for nonlocal Hamiltonian simulation. Third, we use results of majorization theory to explicitly solve the problem of optimal simulation of two-qubit Hamiltonians using LU (equivalently, LU+anc., LO, or LOCC).

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I. INTRODUCTION

The problem of using a given nonlocal Hamiltonian H and some class of local operations to simulate another nonlocal Hamiltonian H' has very recently attracted the attention of several authors in quantum information science [1–7]. Nonetheless, average Hamiltonian techniques, a basic ingredient in nonlocal Hamiltonian simulation, have been studied for many years in control theory [8], and are commonly used in the area of nuclear magnetic resonance [9].

From the perspective of quantum information science, nonlocal Hamiltonian simulation sets a frame for the parametrization of the nonlocal resources contained in multiparticle Hamiltonians, very much in the line of thought pursued to quantify the entanglement of multiparticle quantum states. In the most common setting, fast local unitary operations LU are performed on a series of systems to effectively modify the Hamiltonian H that couples them. A remarkable result is the qualitative equivalence of all bipartite interactions under LU [2,4–7]. This can be shown to imply that any Hamiltonian H with pairwise interactions between some of the systems can simulate any other Hamiltonian H' consisting of arbitrary pairwise interactions between the same systems.

At a quantitative level, the time efficiency with which a Hamiltonian H is able to simulate a Hamiltonian H' can be used as a criterion to endow the set of nonlocal Hamiltonians with a (pseudo) partial order structure that allows to compare the nonlocal capabilities of H and H' [4]. For two-qubit Hamiltonians, simulations using LU or arbitrary local operations LO have been shown to yield the same optimal time efficiencies, and the resulting partial order structure has been computed explicitly. This has led to the necessary and sufficient conditions for H to be able to simulate H' *efficiently* for infinitesimal times, that is, the conditions under which the use of H for time t allows to simulate H' for the same time t, in the small time t limit. Equivalently, this result shows how to *time-optimally* simulate H' with H, in the sense of achieving the maximal simulation ratio t'/t, where t is the time of interaction H that it takes to simulate interaction H' for a time t'.

A. Ancillary systems, generalized local measurements, and classical communication in nonlocal Hamiltonian simulation

The aim of this paper is to elucidate the role a number of resources play in the simulation of nonlocal Hamiltonians. Relatedly, we seek to establish equivalences between different classes of operations that may be used in a simulation protocol.

We first address the question whether classical communication (CC) between the systems is useful in nonlocal Hamiltonian simulation. Recall that in protocols that include local measurements, the ability to communicate which outcome has been obtained in measuring one of the systems allows for subsequent operations on other systems to depend on this information. Now, can this ability be used in nonlocal Hamiltonian simulation to enlarge the set of achievable simulations? Suggestively enough, the answer is yes in the closely related problem of converting one nonlocal gate into another nonlocal gate using LO. For instance, a series of two-qubit gates U exist such that they can be achieved by performing a Controlled-NOT gate and LOCC but cannot be achieved by a Controlled-NOT gate and LO [10].

We also study the advantage of using ancillary systems in simulation protocols, as well as performing general local operations instead of just local unitary transformations. Altogether, our analysis refers to the following classes of transformations: (a) local unitary operations (LU), (b) local unitary operations with ancillas (LU+anc.), (c) local operations (LO) [11], and (d) local operations with classical communication (LOCC).

B. Results

This paper contains the following three main results concerning the simulation of nonlocal Hamiltonian evolutions for infinitesimal times.

(i) LOCC (or LO) simulation protocols can be reduced to LU+anc. simulation protocols. That is, for N-particle Hamiltonian interactions H and H', any protocol that simulates H' using H and LOCC (or LO) can be replaced, without changing its time efficiency, with a protocol involving only H and local unitary transformations. Each local unitary transformation may be performed jointly on one of the N systems and a local ancilla.

(ii) Apart from exceptional cases such as that of two-qubit Hamiltonians [4]—in which any LU+anc. protocol can be further replaced with an even simpler protocol that uses only LU on each qubit— the use of ancillas is, in general, advantageous. This is proven by constructing explicit examples of LU+anc. protocols where ancillas are used to obtain simulations that cannot be achieved with only LU operations, both in the case of two d-level systems ($d>2$) and in the case of $N>2$ systems.

(iii) For two-qubit Hamiltonians, we use results of majorization theory to recover the optimality results presented in Ref. [4]. In view of the equivalence between LU, LU+anc., LO, and LOCC protocols for two-qubit systems, this solves the problem of time optimal, two-qubit Hamiltonian simulation under any of these classes of operations.

The structure of the paper is as follows. In Sec. II we introduce some known results. Sections III, IV, and V present results (i), (ii), and (iii), respectively. Section VI contains some conclusions and Appendixes A and B discuss some technical aspects of Secs. III and V.

II. PRELIMINARIES

We start by reviewing some background material from Ref. [4], of which the present work can be regarded as an extension.

A. Nonlocal Hamiltonian simulation and classes of operations

Recall that the aim of nonlocal Hamiltonian simulation is, given a set of systems that interact according to Hamiltonian H for time t and a class C of local control operations, to be able to produce an evolution $e^{-iH't'}$ for the systems, where H' and t' are the simulated Hamiltonian and the simulated time. (We take $\hbar\equiv 1$ along the paper.)

As mentioned above, one can consider several classes of operations to assist in the simulation, including LU, LU +anc., LO, and LOCC. As in Ref. [4], we make two basic assumptions: (i) these additional operations can be implemented very fast compared to the time scale of the Hamiltonian H (we actually consider the setting in which they can be performed *instantaneously* and thus characterize the fast control limit); (ii) these operations are a cheap resource, so that optimality over simulation protocols is defined only in terms of the ratio t'/t, that is, in terms of how much time t' of evolution according to H' can be produced by using H for a time t. Another interesting parameter characterizing simulations, which we do not analyze here, would be some measure of the complexity of the simulation, that is, of the number of control operations that are performed.

We also note that the inclusions between classes of operations, LU $\subset$ LU+anc. $\subset$ LO $\subset$ LOCC, imply relations between the sets of achievable simulations and time efficiencies. For instance, since LOCC simulation protocols strictly contain all LU simulation protocols, we expect that LOCC protocols may be more powerful than LU protocols.

B. Infinitesimal-time simulations

The maximal simulation factor $s(t')\equiv t'/t$ when simulating $e^{-iH't'}$ by using H for time t may depend on t'. However, we are ultimately interested in characterizing the nonlocal properties of interaction Hamiltonians, irrespective of interaction times. A sensible way to proceed is by considering the worst case situation, namely, the time t' for which the optimal ratio $s(t')$ achieves its minimal value. This occurs for an infinitesimal time t'. That is, simulations of H' for a time such that $||H't'||\ll 1$ are, comparatively, the most expensive in terms of the required time t of interaction H. The reason is that, (i) simulations for an infinitesimal time are a particular case of simulation, providing an upper bound for the minimum of $s(t')$, and (ii) any finite-time simulation—or *gate synthesis*—can be achieved, maybe not optimally, by concatenating infinitesimal-time simulations.

We shall denote $s_{H'|H}$ the limit $\lim_{t'\to 0} s(t')$, and call it the simulation factor of H' with H ($s_{H'|H}$ corresponds to the inverse of the time overhead μ of Ref. [3], that is, $s_{H'|H}=\mu^{-1}$). Then, apart from quantifying the time efficiency in infinitesimal simulations, $s_{H'|H}$ has also two other meanings.

(1) $T'/s_{H'|H}$ upper bounds the time T of use of H needed to perform the unitary gate $e^{-iH'T'}$, for any T' (*gate simulation* or *gate synthesis* [13]).

(2) $s_{H'|H}$ is the optimal time efficiency in *dynamics simulation*. That is, $s_{H'|H}$ is the maximal achievable ratio T'/T, where T is the time of H required to simulate the *entire* evolution of a system according to $e^{-it'H'}$, where t' runs from 0 to T' [12].

In an abuse of notation, we shall refer to condition $||H't'||\ll 1$ as the small time limit, of which $O(t')$ [or $O(t)$] will denote the first order corrections.

C. Optimal and efficient simulations

For any class $C\in$ {LU, LU+anc., LO, LOCC} of the above operations and in the small time limit, the space of achievable evolutions using Hamiltonian H and operations C turns out to be convex. Then the following two problems (P1) given any H and H', determine when H' can be efficiently (i.e., $t'=t$) simulated with H for infinitesimal times, denoted

$$H'\leqslant_C H; \tag{1}$$

(P2) given any H and H', determine the simulation factor $s_{H'|H}$; are equivalent, since $s_{H'|H}$ is nothing but the greatest s such that sH' can be efficiently simulated by H, that is, such that $sH'\leqslant_C H$.

D. Equivalence of LO and LU+anc. protocols

The simulation of nonlocal Hamiltonians using LO and that using LU+anc. are equivalent (see Ref. [4] for details),

in that any protocol based on LO can be replaced with another one that uses only LU+anc. and that has the same time efficiency. The ultimate reason for this equivalence is that even if LO provide, through measurement outcomes, information that can be used to decide on posterior local manipulations, this information cannot be transmitted to the other parties (unless the interaction itself is used for this purpose, but this leads to null efficiency t'/t when $t\to 0$); then, unitarity of the simulated evolution implies that each party is effectively applying a trace-preserving local operation on its subsystem, and this can always be achieved using only LU +anc.

The previous situation changes when classical communication is allowed between the parties, because then they can coordinate their manipulations. In spite of this fact, CC does not help in Hamiltonian simulation, as we move to discuss next.

III. EQUIVALENCE OF LOCC AND LU+anc. PROTOCOLS

In this section we show that any protocol for nonlocal Hamiltonian simulation based on LOCC can be replaced with another one based only on LU+anc. and having the same time efficiency. This result, valid for infinitesimal-time simulations on arbitrary N-particle systems, brings an important simplification to the general problem of nonlocal Hamiltonian simulation, since it implies the equivalence of LOCC, LO, and LU+anc. protocols.

We first describe in detail the most general protocol for Hamiltonian simulation using LOCC. Then we show—through an argument that exploits the fact that entanglement only decreases under LOCC—that any such protocol can be replaced with another one using only LU+anc. The key point of the proof is to assume that one of the systems is initially entangled with an auxiliary system Z, and to realize that a nontrivial measurement (i.e., a measurement not equivalent to some local unitary transformation) on the system would partially destroy this entanglement in an irreversible way. Since we are simulating a unitary process on the systems (which should preserve the entanglement between those and Z), all local measurements must be trivial, and can be replaced with unitary transformations.

A. Hamiltonian simulation using LOCC

For the sake of clarity we will perform most of the analysis in the simplest nontrivial case, that involving only two qubits, because this already contains all the ingredients of the general N-particle setting. Let us consider, then, that qubits A and B, with Hilbert spaces $\mathcal{H}_A$ and $\mathcal{H}_B$, interact according to H for an overall time t, and that, simultaneously, they are being manipulated locally.

1. Local manipulation

The most general local operation on, say, qubit A can be achieved by (i) appending to A an ancillary system A' in some blank state $|0_{A'}\rangle\in\mathcal{H}_{A'}$; (ii) performing a unitary transformation U on $\mathcal{H}_{AA'}=\mathcal{H}_A\otimes\mathcal{H}_{A'}$; (iii) performing an orthogonal measurement on a factor space $\mathcal{H}_{meas}$ of the total Hilbert space $\mathcal{H}_{AA'}=\mathcal{K}\otimes\mathcal{H}_{meas}$, given by projection operators $\{P^\beta\}$; and (iv) tracing out a factor space $\mathcal{T}^\beta$ of $\mathcal{H}_{AA'}=\mathcal{H}_{out}^\beta\otimes\mathcal{T}^\beta$, where $\mathcal{H}_{out}^\beta$ and $\mathcal{T}^\beta$ may depend on the measurement outcome β of step (iii). Under (i)–(iv) the initial state $|\phi_A\rangle$ of qubit A transforms with probability p_β according to

$$|\phi_A\rangle\langle\phi_A|\to\mathcal{E}_\beta(|\phi_A\rangle\langle\phi_A|)=\frac{1}{p_\beta}\mathrm{tr}_{\mathcal{T}^\beta}[P^\beta U(|\phi_A\rangle\langle\phi_A|\otimes|0_{A'}\rangle\times\langle 0_{A'}|)U^\dagger P^\beta], \tag{2}$$

where $p_\beta\equiv\mathrm{tr}[P^\beta U(|\phi_A\rangle\langle\phi_A|\otimes|0_{A'}\rangle\langle 0_{A'}|)U^\dagger P^\beta]$. We can introduce operators $M_i^\beta:\mathcal{H}_A\to\mathcal{H}_{out}^\beta$,

$$M_i^\beta\equiv\langle i^\beta|P^\beta U|0_{A'}\rangle, \tag{3}$$

where $\{|i^\beta\rangle\}$ is an orthonormal basis of $\mathcal{T}^\beta$. Then Eq. (2) can be rewritten as

$$\mathcal{E}_\beta(|\phi_A\rangle\langle\phi_A|)=\frac{1}{p_\beta}\sum_i M_i^\beta|\phi_A\rangle\langle\phi_A|M_i^{\beta\dagger}. \tag{4}$$

Now, since in our case the eventual result of this manipulation must be a unitary evolution, we are interested in transformations $\mathcal{E}_\beta$ that map pure states into pure states, that is, such that can be implemented by just one operator $M^\beta:\mathcal{H}_A\to\mathcal{H}_{out}^\beta$,

$$|\phi_A\rangle\langle\phi_A|\to\frac{1}{p_\beta}M^\beta|\phi_A\rangle\langle\phi_A|M^{\beta\dagger}, \tag{5}$$

$p_\beta=\mathrm{tr}[M^\beta|\phi_A\rangle\langle\phi_A|M^{\beta\dagger}]$. Therefore the effect of the local manipulation on qubit A is a generalized measurement $\mathcal{M}$ that, with probability p^β, maps the state of A into a state supported on $\mathcal{H}_{out}^\beta$,

$$|\phi_A\rangle\to\frac{1}{\sqrt{p^\beta}}M^\beta|\phi_A\rangle, \tag{6}$$

and produces classical information β. The measurement operators $\{M^\beta\}$ characterizing $\mathcal{M}$ satisfy $\Sigma_\beta M^{\beta\dagger}M^\beta=I_A$.

More generally, in a simulation protocol measurement $\mathcal{M}$ may depend on some previous information α, in which case we write $\mathcal{M}^\alpha$. In addition, the corresponding measurement operators $\{M^{\beta,\alpha}\}$ may map states from a two-dimensional subspace $\mathcal{H}_{in}^\alpha\subset\mathcal{H}_{AA'}$ into another two-dimensional subspace $\mathcal{H}_{out}^{\beta,\alpha}\subset\mathcal{H}_{AA'}$ that depends both on the measurement outcome β and on the previous information α, that is,

$$M^{\beta,\alpha}:H_{in}^\alpha\to H_{out}^{\beta,\alpha}. \tag{7}$$

In the following, a series of measurements $\mathcal{M}$ will be concatenated, in such a way that the *out subspace* $\mathcal{H}_{out}$ for a given measurement is related to the *in subspace* $\mathcal{H}_{in}$ for the next one.

We consider that a sufficiently large ancillary system A' in a pure state has been initially appended to qubit A so that it provides at once the extra degrees of freedom needed to perform all generalized measurements $\mathcal{M}$ on A. Finally, all the above considerations apply also to qubit B, to which an ancillary system B' is appended.

2. LOCC simulation protocol

A LOCC protocol for simulating $e^{-it'H'}$ by H for time t is characterized by a partition $\{t_1,t_2,\ldots,t_n\}$ of t, where $t_i \geqslant 0$, $\Sigma_i t_i = t$, and a series of local measurements, $\{(\mathcal{M}_0,\mathcal{N}_0),(\mathcal{M}_1^{\alpha_1},\mathcal{N}_1^{\alpha_1}),\ldots,(\mathcal{M}_n^{\alpha_n},\mathcal{N}_n^{\alpha_n})\}$. The protocol runs as follows.

(1) The simulation begins with measurements $\mathcal{M}_0$ and $\mathcal{N}_0$ being performed on A and B, respectively. These map the original state of AB into a state supported on some subspace of $AA'BB'$.

(2) Then the two qubits A and B are left to evolve according to H for a time t_1.

(3) After that, measurements $\mathcal{M}_1^{\alpha_1}$ and $\mathcal{N}_1^{\alpha_1}$ are performed. Here, index α_1 indicates that the measurements being performed after time t_1 may depend on the outcomes of measurements $\mathcal{M}_0$ and $\mathcal{N}_0$.

(4) Again, the measurements are followed by an evolution, for time t_2, of A and B according to H, and the protocol continues in an iterative fashion.

(5) In step k, qubits A and B are first left to evolve according to H for a time t_k and then measurements $\mathcal{M}_k^{\alpha_k}$ and $\mathcal{N}_k^{\alpha_k}$ (α_k denoting again a possible dependence on the outcome of all previous measurements) are locally performed in AA' and BB'.

(6) The protocol finishes after measurements $\mathcal{M}_n^{\alpha_n}$ and $\mathcal{N}_n^{\alpha_n}$ have been performed. These last measurements must leave the two-qubit system AB in a pure state (that is, uncorrelated from systems $A'B'$ that are traced out).

Thus, the two-qubit system AB is initially in some state $|\psi\rangle$, becomes entangled with the ancillas A' and B' during the manipulations described above, but ends up in the state $e^{-iH't'}|\psi\rangle$ after time t.

Note that the protocol described above has a tree structure, starting with a preestablished pair of local manipulations and ending up at the extreme of a branch characterized by the outcomes of all (conditioned) local operations performed during the time interval t. We move now to characterize one of these branches.

3. One branch of the protocol

Let us suppose we run the simulation once. This corresponds to some given branch of the protocol, which we label Γ, and which we have represented in Fig. 1. Branch Γ is characterized by a series of measurement operators $\{(M_0^\Gamma,N_0^\Gamma),\ldots,(M_n^\Gamma,N_n^\Gamma)\}$, where the superindices α_k containing the information that characterizes the branch have been replaced with Γ to simplify the notation. Recall that the aim of the protocol is to achieve an evolution according to

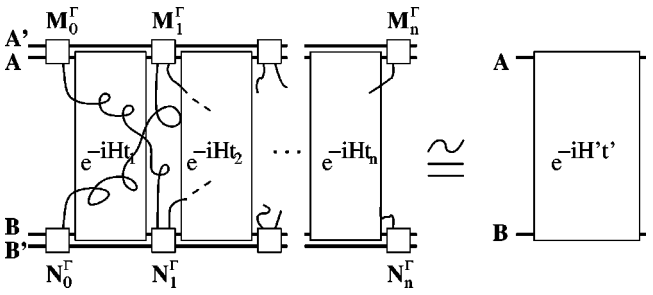

FIG. 1. Schematic representation of a Hamiltonian simulation protocol using LOCC. The unitary evolution of the composite system AB according to H and for a time $t=\Sigma_i t_i$ is interspersed with local measurements $\mathcal{M}_k^{\alpha_k}$ (on systems AA') and $\mathcal{N}_k^{\alpha_k}$ (on systems BB') to obtain a unitary evolution of AB according to H' and for a time t'. Here α_k indicates the local measurements performed at step k, which may depend on the outcome of all previous steps, owing to the classical communication between the systems (winding lines). In the figure we have replaced the superscripts α_k with Γ, Γ denoting a particular branch of the protocol [cf. Eq. (8)]. Thus, in branch Γ measurement operators M_k^Γ (corresponding to measurement $\mathcal{M}_k^\Gamma$) and N_k^Γ (corresponding to measurement $\mathcal{N}_k^\Gamma$) transform systems AA' and BB' at step k of the protocol.

$e^{-iH't'}$. Therefore, for any initial vector $|\psi\rangle$ of the two-qubit system AB, the measurement operators $\{(M_k^\Gamma,N_k^\Gamma)\}_{k=0}^n$ must obey

$$\sqrt{p_\Gamma}e^{-iH't'}|\psi\rangle = (M_n^\Gamma\otimes N_n^\Gamma)e^{-it_nH}\cdots(M_1^\Gamma\otimes N_1^\Gamma)e^{-it_1H}(M_0^\Gamma\otimes N_0^\Gamma)|\psi\rangle, \tag{8}$$

where p_Γ denotes the probability that branch Γ occurs in the protocol. Equation (8) is the starting point for the rest of the analysis in this section.

B. LOCC protocols are as efficient as LU+anc. protocols for infinitesimal-time simulations

As discussed in the Introduction, we are interested here in simulations for an infinitesimal simulation time t. In this regime Eq. (8) significantly simplifies, because we can expand the exponentials to first order in t (or equivalently, in $\{t_k\}$ and t'), thereby obtaining an equation that is linear both in H and H'. In addition, if t is small then qubits A and B interact only "a little bit." In what follows we will use this fact to prove the main result of this section, namely, that all the measurement operators $\{M_k^\Gamma,N_k^\Gamma\}_{k=0}^n$ in Eq. (8) must be, up to negligible corrections, proportional to unitary operators in some corresponding relevant supports. This will eventually imply that LU+anc. protocols can already simulate any evolution $e^{-iH't'}$ achievable in a LOCC protocol.

We note that this result is not valid for the interconversion of nonlocal gates [10]. There the systems are allowed to interact according to a finite gate (e.g., a Controlled-NOT gate), and thus accumulate some finite amount of entanglement (e.g., an *ebit*) in the ancillary systems, that can be used, together with LOCC, to perform some new nonlocal gate (e.g., through some teleportation scheme).

1. LOCC protocols for infinitesimal-time simulations

We define a series of operators M_k and M'_k by

$$M_k \equiv M_n^\Gamma \cdots M_k^\Gamma, \qquad k=1,\ldots,n,$$

$$M'_k \equiv M_{k-1}^\Gamma \cdots M_0^\Gamma, \qquad k=1,\cdots,n,$$

$$M_0 \equiv M_n^\Gamma \cdots M_0^\Gamma, \tag{9}$$

and also an analogous series of operators N_k, N'_k, and N_0. Notice that operator M'_k describes a concatenation of all local measurements in branch Γ performed from the beginning of the protocol and up to step $k-1$ on the state initially supported on $\mathcal{H}_{AA'}$, while M_k collects the manipulations that will be performed from step k until the end of the protocol. In the small time regime, we can expand the exponentials in Eq. (8) as a series in t_k and t' to obtain, up to second order corrections $O(t^2)$,

$$\sqrt{p_\Gamma}(I_{AB}-istH')|\psi\rangle = \Big(M_0\otimes N_0 - it\sum_{k=1}^{n} p_k (M_k\otimes N_k) \times H(M'_k\otimes N'_k)\Big)|\psi\rangle, \tag{10}$$

where we have introduced probabilities $p_k \equiv t_k/t$ and the efficiency factor $s\equiv t'/t$ of the branch, so that all times are expressed in terms of t.

This equation indicates that

$$M_0\otimes N_0|\psi\rangle = \sqrt{p_\Gamma} I_{AB}|\psi\rangle + O(t), \tag{11}$$

for any two-qubit state $|\psi\rangle$, from which it follows that the probability p_Γ that branch Γ occurs cannot depend on $|\psi\rangle$ up to $O(t)$ corrections, also that both M_0 and N_0 must be proportional to the identity operator in H_A and H_B,

$$M_0 = \sqrt{p_\Gamma} q I_A + O(t), \tag{12}$$

$$N_0 = q^{-1} I_B + O(t), \tag{13}$$

where q is some positive parameter. Notice that the order t corrections in Eq. (11) correspond to local terms, that is, to operators of the form $t(I_A\otimes O_B + O'_A\otimes I_B)$, and thus are irrelevant to this discussion [14]. In what follows we neglect these local terms for the sake of clarity. Bearing this remark and Eq. (11) in mind, we rewrite Eq. (10) as the operator equation

$$\sqrt{p_\Gamma}(I_{AB}-istH') = \sqrt{p_\Gamma} I_{AB} - it\sum_{k=1}^{n} p_k (M_k\otimes N_k) \times H(M'_k\otimes N'_k) + O(t^2). \tag{14}$$

That is,

$$\sqrt{p_\Gamma} sH' = \sum_{k=1}^{n} p_k (M_k\otimes N_k) H(M'_k\otimes N'_k) + O(t), \tag{15}$$

where, because of Eq. (11), some other constraints apply. More precisely, if M'_k and N'_k are given by

$$M'_k = \sqrt{p_\Gamma} q(|\mu_0^k\rangle\langle 0_A| + |\mu_1^k\rangle\langle 1_A|),$$

$$N'_k = q^{-1}(|\nu_0^k\rangle\langle 0_B| + |\nu_1^k\rangle\langle 1_B|), \tag{16}$$

where $\{|i_A\rangle\}$ and $\{|i_B\rangle\}$ are orthonormal bases of $\mathcal{H}_A$ and $\mathcal{H}_B$ and $\{|\mu_i^k\rangle \in \mathcal{H}_{AA'}\}$ and $\{|\nu_i^k\rangle \in \mathcal{H}_{BB'}\}$ are arbitrary vectors, not necessarily normalized, then M_k and N_k must fulfill

$$M_k = |0_A\rangle\langle\tilde{\mu}_0^k| + |1_A\rangle\langle\tilde{\mu}_1^k| + O(t),$$

$$N_k = |0_B\rangle\langle\tilde{\nu}_0^k| + |1_A\rangle\langle\tilde{\nu}_1^k| + O(t), \tag{17}$$

where $\{|\tilde{\mu}_i^k\rangle\}$ is the biorthonormal basis [15] of $\{|\mu_i^k\rangle\}$ (in the subspace spanned by $\{|\mu_i^k\rangle\}$), that is, $\langle\mu_i^k|\tilde{\mu}_j^k\rangle = \delta_{ij}$, and similarly $\{|\tilde{\nu}_i^k\rangle\}$ is the biorthonormal basis of $\{|\nu_i^k\rangle\}$, so that $M_0\otimes N_0 = (M_k M'_k)\otimes(N_k N'_k)$ fulfills Eq. (11).

Now, going back to the measurement operators M_k^Γ, we can expand them as

$$M_0^\Gamma = \sqrt{p_\Gamma} q(|\mu_0^1\rangle\langle 0_A| + |\mu_1^1\rangle\langle 1_A|),$$

$$M_k^\Gamma = |\mu_0^{k+1}\rangle\langle\tilde{\mu}_0^k| + |\mu_1^{k+1}\rangle\langle\tilde{\mu}_1^k|, \qquad k=1,\ldots,\ n-1$$

$$M_n^\Gamma = |0_A\rangle\langle\tilde{\mu}_0^n| + |1_A\rangle\langle\tilde{\mu}_1^n| + O(t), \tag{18}$$

and similarly for the N_k^Γ.

2. Unitarity and conservation of entanglement

We carry on this analysis by focusing our attention only on the operations performed on systems AA'. We will show that operators M_k and M'_k can be replaced with operators proportional to $\langle 0_{A'}|U_k$ and $U_k^\dagger|0_{A'}\rangle$, where U_k is a unitary matrix acting on $H_{AA'}$. We will use the fact that the protocol must be able to keep the entanglement of A with another system Z.

Let us suppose, then, that qubit A is entangled with a distant qubit Z, with the maximally entangled vector

$$\frac{1}{\sqrt{2}}(|0_A\rangle\otimes|0_Z\rangle + |1_A\rangle\otimes|1_Z\rangle) \tag{19}$$

describing the pure state of AZ. Any unitary evolution of qubits A and B preserves the amount of entanglement between qubit Z and qubits AB. In particular, if the unitary evolutions according to H are infinitesimal, then up to $O(t)$ corrections qubit Z must be still in a maximally entangled state with A after the simulated evolution $e^{-istH'}$. This sets very strong restrictions on the kind of measurements that can be performed on A during the simulation protocol. If during the k^{th} measurement in branch Γ part of the entanglement is destroyed, then the simulation protocol necessarily fails with some probability, because the destroyed entanglement cannot be deterministically recovered. Indeed, even if subsequent measurement operators in branch Γ would be able to restore

the entanglement and so obey Eq. (8), another branch Γ' diverging from Γ after the kth measurement must necessarily fail to recover the entanglement (recall the monotonically decreasing character of entanglement under LOCC, see, e.g., Ref. [16]) and thus with some probability the protocol must fail to simulate the unitary evolution [17].

Let us see the effect of this restriction on the first measurement operator M_0^Γ in Eq. (18). It transforms the initial entangled state into a new state proportional to

$$|\mu_0^1\rangle\otimes|0_Z\rangle+|\mu_1^1\rangle\otimes|1_Z\rangle, \tag{20}$$

which remains maximally entangled if and only if $|||\mu_0^1\rangle||=|||\mu_1^1\rangle||\equiv r_1$ and $\langle\mu_0^1|\mu_1^1\rangle=0$. But this is precisely the condition for $M_1'(=M_0^\Gamma)$ to be proportional to a unitary operator from $\mathcal{H}_A$ to the out space $\mathcal{H}_{out}^0$ spanned by $\{|\mu_i^1\rangle\}$ or, equivalently, to an isometry from $\mathcal{H}_A$ to $\mathcal{H}_{AA'}$. Thus, we can write

$$M_1'=r_1U_1^\dagger|0_{A'}\rangle, \tag{21}$$

where

$$U_1^\dagger\equiv\frac{|\mu_0^1\rangle}{r_1}\langle 0_A0_{A'}|+\frac{|\mu_1^1\rangle}{r_1}\langle 1_A0_{A'}|+\sum_{l=1}^{d_{A'}-1}|\xi_{l,0}\rangle\langle 0_Al_{A'}| +|\xi_{l,1}\rangle\langle 1_Al_{A'}|$$

is some unitary operation defined on $\mathcal{H}_{AA'}$. Here $d_{A'}$ is the dimension of $\mathcal{H}_{A'}$ and $\{|\xi_{l,0}\rangle,|\xi_{l,1}\rangle\}_{l=1}^{d_{A'}}$ is some set of vectors that together with $|\mu_0^1\rangle/r_1$ and $|\mu_1^1\rangle/r_1$ form an orthonormal basis of $\mathcal{H}_{AA'}$. Equation (17) implies that, in addition,

$$M_1=\frac{\sqrt{p_\Gamma}q}{r_1}\langle 0_{A'}|U_1. \tag{22}$$

This characterization in terms of a unitary transformation can now be easily extended to the rest of operators M_k and M_k'. We use induction over k. We already have that the characterization works for $k=1$. Suppose it works for some $k-1$, that is, in the decomposition Eq. (16) for M_{k-1}' we have $|||\mu_0^{k-1}\rangle||=|||\mu_1^{k-1}\rangle||$ and $\langle\mu_0^{k-1}|\mu_1^{k-1}\rangle=0$. This means that after the $(k-1)^{\text{th}}$ measurement in branch Γ, the initial state of Eq. (19) becomes a state proportional to

$$|\mu_0^{k-1}\rangle\otimes|0_Z\rangle+|\mu_1^{k-1}\rangle\otimes|1_Z\rangle+O(t), \tag{23}$$

where the $O(t)$ corrections are due to evolutions of AB according to H for a time of order t, which slightly entangle B with AZ. Then, preservation of entanglement during the k^{th} measurement (implemented by operator M_{k-1}^Γ) requires that also $|||\mu_k^0\rangle||=|||\mu_k^1\rangle||\equiv r_k$ and $\langle\mu_k^0|\mu_k^1\rangle=0$, and therefore

$$M_k'=r_kU_k^\dagger|0_{A'}\rangle+O(t),$$

$$M_k=\frac{\sqrt{p_\Gamma}q}{r_k}\langle 0_{A'}|U_k+O(t), \tag{24}$$

for some unitary transformation U_k acting on $\mathcal{H}_{AA'}$.

The same argument leads to expressing the operators N_k and N_k' in terms of unitary transformations V_k acting on $\mathcal{H}_{BB'}$ as

$$N_k'=s_kV_k^\dagger|0_{B'}\rangle+O(t),$$

$$N_k=\frac{1}{r_kq}\langle 0_{B'}|V_k+O(t). \tag{25}$$

Therefore Eq. (15) finally reads, up to $O(t)$ corrections that vanish in the $t\to 0$ or fast control limit,

$$sH'=\sum_k p_k\langle 0_A,0_{B'}|(U_k\otimes V_k)H(U_k^\dagger\otimes V_k^\dagger)|0_A,0_{B'}\rangle. \tag{26}$$

3. Equivalence between LOCC and LU+anc. protocols

The set S_H^{LOCC} of nonlocal Hamiltonians that can be efficiently simulated by H and LOCC is *convex*: if H can efficiently simulate H_1 and H_2, then it can also efficiently simulate the Hamiltonian $pH_1+(1-p)H_2$. Indeed, we just need to divide the infinitesimal time t into two parts and simulate H_1 for time pt and then H_2 for time $(1-p)t$. The resulting Hamiltonian is precisely the above average of H_1 and H_2. Thus, in order to characterize the convex set S_H^{LOCC}, we can focus on its *extreme points*. Notice that the previous convexity argument also holds for the set $S_H^{LU+anc.}$ of Hamiltonians that can be efficiently simulated with LU+anc., so that $S_H^{LU+anc.}$ is also convex. Recall also that $S_H^{LU+anc.}\subset S_H^{LOCC}$.

Now, Eq. (26) says that all points in S_H^{LOCC} can be obtained as a convex combination of terms of the form

$$\langle 0_A,0_{B'}|(U\otimes V)H(U^\dagger\otimes V^\dagger)|0_A,0_{B'}\rangle. \tag{27}$$

In addition, in Appendix A we show that any such term can be obtained in a simulation protocol using LU+anc. It follows that (i) any extreme point of S_H^{LOCC} is of the form (27), and that (ii) any extreme point of S_H^{LOCC} belongs to $S_H^{LU+anc.}$, so that $S_H^{LU+anc.}=S_H^{LOCC}$. This finishes the proof of the fact that infinitesimal-time simulations using LOCC can always be accomplished using LU+anc.

Summarizing, we have seen that any (rescaled) two-qubit Hamiltonian sH' achievable in branch Γ of our LOCC-simulation protocol [cf. Eq. (26)] can also be achieved, with the same time efficiency, by just using local unitary transformations and ancillas as extra resources. It is now straightforward to generalize the above argument to N systems, each one having two or more levels, thereby extending the equivalence of LOCC and LU+anc. protocols to general multiparticle interactions. Indeed, for any d-level system involved in the simulation, we just need to require that its entanglement with some remote, auxiliary d-level system be preserved, and we readily obtain that all measurements performed during the simulation protocol can be replaced with local unitary operations. We thus can conclude, using the notation introduced in Sec. II B, that

$$H'\leqslant_{LOCC}H\Leftrightarrow H'\leqslant_{LU+anc.}H. \tag{28}$$

IV. LU+anc. PROTOCOLS ARE NOT EQUIVALENT TO LU PROTOCOLS

The equivalence between infinitesimal-time simulations using LOCC and LU+anc. may be conceived as a satisfactory result. On the one hand, it discards local measurements and classical communication as useful resources for the simulation of nonlocal Hamiltonians. This essentially says that in order to simulate Hamiltonian dynamics, we can restrict the external manipulation to unitary operations, possibly involving some ancillary system. In this way the set of interesting simulation protocols has been significantly simplified. On the other hand, it is reassuring to see that, despite the diversity of classes of operations that we may use as a criterion to characterize the nonlocal properties of multiparticle interactions, most of these criteria (LOCC, LO, and LU +anc.) yield an equivalent classification and quantification. In other words, we do not have to deal with a large number of alternative characterizations. We shall show here, however, that simulation using only LU, that is, without ancillas, is not equivalent to that using LU+anc.

The reason for this inequivalence is the following. Consider a multipartite Hamiltonian of the form $H_A \otimes H_{BC\cdots}$, where H_A acts on a d-dimensional space $\mathcal{H}_A$ and $H_{BC\cdots}$ acts on $\mathcal{H}_B \otimes \mathcal{H}_C \cdots$. In the presence of an ancilla $\mathcal{H}_{A'}$, LU can be used so that operator H_A acts on some d-dimensional *factor* space $\mathcal{K}$ of $\mathcal{H}_{AA'}$ $(\mathcal{H}_{AA'} = \mathcal{K} \otimes \mathcal{K}')$. The net result is an effective Hamiltonian acting on $\mathcal{H}_A$. As the following examples show, some of these effective Hamiltonians cannot be achieved (at least with the same time efficiencies) by using only LU.

A. LU+anc. protocols versus LU protocols

In the preceding section we saw that, in the fast control limit, the extreme points of the convex set $S_H^{LU+anc.}$ of bipartite Hamiltonians that can be efficiently simulated with H using LU+anc. (equivalently, those of the set S_H^{LOCC}) are, up to local terms, of the form

$$\mathcal{E}(H) \equiv \langle 0_{A'} 0_{B'} | U \otimes V (H \otimes I_{A'B'}) U^\dagger \otimes V^\dagger | 0_{A'} 0_{B'} \rangle \tag{29}$$

(an analogous expression holds for the multipartite case). Notice that in Eq. (29) we have replaced operator H of Eq. (27) with $H \otimes I_{A'B'}$ to make more explicit that ancillas are being used.

Can all simulations of this type be achieved by using only LU? The most general simulation that can be achieved from H and by LU reads (see Ref. [4] for more details)

$$\sum_k p_k u_k \otimes v_k H u_k^\dagger \otimes v_k^\dagger + m \otimes I_B + I_A \otimes n + a I_{AB}, \tag{30}$$

where $\{p_k\}$, $\Sigma_k p_k = 1$, is a probability distribution, $\{u_k\}$ and $\{v_k\}$ are local unitaries acting on A and B, m and n are self-adjoint, traceless operators, and a is a real constant. The previous question translates then into whether for any U and V in Eq. (29), we can find a set $\{p_k, u_k, v_k\}$, m, n, and a such that Eq. (30) equals $\mathcal{E}(H)$ in Eq. (29).

In Ref. [4] it was shown that, in the particular case of two-qubit systems, the previous conditions can always be fulfilled. Next we shall show that this is sometimes not the case for Hamiltonians of two d-level systems for $d > 2$, and also for Hamiltonians of more than two systems.

B. Inequivalence between LU+anc. and LU protocols

1. Example 1: Two d-level systems ($d > 2$)

We first consider two d-level systems A and B, $d > 2$, that interact according to

$$K \equiv P_0 \otimes P_0 + \sum_{i=1}^{d-1} P_i \otimes P_i, \tag{31}$$

where $P_i \otimes P_j \equiv |i_A\rangle\langle i_A| \otimes |j_B\rangle\langle j_B|$. We will show that by means of LU+anc., Hamiltonian K can be used to efficiently (that is, with unit efficiency factor s) simulate

$$K' \equiv P_0 \otimes P_1 + \sum_{i=1}^{d-1} P_i \otimes P_i. \tag{32}$$

We will also show that K' cannot be efficiently simulated using only LU.

Let A' be a d-level ancilla. We need a unitary transformation U satisfying

$$\langle 0_{A'} | U = |0_A\rangle\langle 1_A 0_{A'}| + \sum_{i=1}^{d-1} |i_A\rangle\langle i_A i_{A'}|. \tag{33}$$

As we discuss in Appendix A, the transformation of a Hamiltonian H acting on AB,

$$\mathcal{E}(H) \equiv \langle 0_{A'} 0_{B'} | U (H \otimes I_{A'B'}) U^\dagger | 0_{A'} 0_{B'} \rangle, \tag{34}$$

can be achieved using LU+anc. [notice that this corresponds to choosing $V_{BB'} = I_{BB'}$ in Eq. (A1)]. In particular, this transformation takes any term of the form $P_i \otimes P_j$ into

$$\mathcal{E}(P_i \otimes P_j) = \begin{cases} 0, & i = 0, \\ (P_0 + P_1) \otimes P_j, & i = 1, \\ P_i \otimes P_j, & i > 1, \end{cases} \tag{35}$$

which in particular implies

$$\mathcal{E}(K) = K'. \tag{36}$$

Now, if this simulation is to be possible with the same time efficiency by using only LU, then we must have, because of Eq. (30),

$$K' = Q + m \otimes I_B + I_A \otimes n + a I_{AB}, \tag{37}$$

where $Q \equiv \Sigma_{i=0}^{d-1} \Sigma_k p_k u_k P_i u_k^\dagger \otimes v_k P_i v_k^\dagger \geq 0$, but this is not possible. Indeed, we first notice that, by taking the trace of this expression we obtain $a = 0$, whereas by tracing out only system B we obtain

$$I = I + dm, \tag{38}$$

and thus $m=0$. Tracing out only system A leads to

$$2P_1+\sum_{i=2}^{d-1} P_i = I+dn, \tag{39}$$

so that $n=(-P_0+P_1)/d$ and condition (37) becomes

$$K'=P_0\otimes P_1+\sum_{i=1}^{d-1} P_i\otimes P_i = Q+\frac{I_A}{d}\otimes(-P_0+P_1). \tag{40}$$

Then, recalling the positivity of Q, we obtain the following contradiction:

$$\begin{aligned} 0 &= \mathrm{tr}[P_2\otimes P_1 K'] \\ &= \mathrm{tr}[P_2\otimes P_1 Q] \\ &\quad + \mathrm{tr}\left[(P_2\otimes P_1)\left(\frac{I_A}{d}\otimes(-P_0+P_1)\right)\right] \\ &= \mathrm{tr}[(P_2\otimes P_1)Q]+1/d \geqslant 1/d. \end{aligned} \tag{41}$$

Thus, for any $d>2$, we have explicitly constructed an example of LU+anc. simulation for Hamiltonians acting on two d-level systems that cannot be achieved using only LU. We recall, however, that for two-particle Hamiltonians, LU +anc. and LU protocols only differ quantitatively, for LU protocols are able to simulate any bipartite Hamiltonian H' starting from any other H with nonvanishing $s_{H'|H}$ [2,4,7].

2. Example 2: A 2×2×2 composite system

Let us consider now the simulation, for an infinitesimal time t, of the three-qubit Hamiltonian

$$K'\equiv I\otimes\sigma_3\otimes\sigma_3, \tag{42}$$

by the Hamiltonian

$$K\equiv\sigma_3\otimes\sigma_3\otimes\sigma_3, \tag{43}$$

where

$$\sigma_3\equiv\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}. \tag{44}$$

This is possible, when allowing for LU+anc. operations, by considering the transformation U acting on qubit A and on a one-qubit ancilla A' in state $|0_{A'}\rangle$, where

$$\langle 0_{A'}|U=|0_A\rangle\langle 0_A|\otimes\langle 0_{A'}|+|1_A\rangle\langle 0_A|\otimes\langle 1_{A'}|. \tag{45}$$

Indeed, we have that $\langle 0_{A'}|U(\sigma_3\otimes I_{A'})U^\dagger|0_{A'}\rangle=I_A$, so that

$$\langle 0_{A'}|UKU^\dagger|0_{A'}\rangle=K'. \tag{46}$$

On the other hand it is impossible to simulate K' by K and LU, for it would imply to transform σ_3 into I through unitary mixing, which is a trace-preserving operation. It is straightforward to construct similar examples in higher-dimensional systems, and also with more than three systems.

We note that, as far as interactions involving more than two systems are concerned, the inequivalence between LU +anc. and LU simulation protocols is not only quantitative, leading to different simulation factors, but also qualitative. The last example above shows that LU protocols cannot be used to simulate Hamiltonians that can be simulated using LU+anc. and the same interaction H.

V. OPTIMAL SIMULATION OF TWO-QUBIT HAMILTONIANS USING LOCC

In this section we address the problem of optimal Hamiltonian simulation using LU for the case of two-qubit interactions. We recover the results of Ref. [4], but through an alternative, simpler proof, based on known results of majorization theory—and thus avoiding the geometrical constructions of the original derivation [4]. The equivalence of LOCC and LU+anc. strategies presented in Sec. III, together with that of LU+anc. and LU strategies for two-qubit Hamiltonians proved in Ref. [4], imply that these results are also optimal in the context of LOCC, LO, and LU+anc. Hamiltonian simulation.

We start by recalling some basic facts. Any two-qubit Hamiltonian H is equivalent, as far as LU simulation protocols are concerned, to its canonical form [1,4]

$$H=\sum_{i=1}^{3} h_i\sigma_i\otimes\sigma_i, \tag{47}$$

where $h_1\geqslant h_2\geqslant|h_3|\geqslant 0$ and the operators σ_i are the Pauli matrices,

$$\sigma_1\equiv\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix},\quad \sigma_2\equiv\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix},\quad \sigma_3\equiv\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}. \tag{48}$$

A brief justification for this canonical form is as follows. Any two-qubit Hamiltonian

$$H_A\otimes I_B+I_A\otimes H_B+\sum_{ij} h_{ij}\sigma_i\otimes\sigma_j \tag{49}$$

can efficiently simulate (or be efficiently simulated by) its canonical form (47): on the one hand we can always use traceless operators m and n as in Eq. (30) to remove (or introduce) the local operators H_A and H_B; then the remaining operator $\Sigma_{ij}h_{ij}\sigma_i\otimes\sigma_j$ can be taken into the canonical form by means of one-qubit unitary operations u and v such that $(u\otimes v)\Sigma_{ij}h_{ij}\sigma_i\otimes\sigma_j(u^\dagger\otimes v^\dagger)$ is diagonal when expressed in terms of Pauli matrices. The coefficients h_i in Eq. (47) turn out to be related to the singular values of the matrix h_{ij}.

Therefore we only need to study the conditions for efficient simulation between Hamiltonians which are in a canonical form. Let $\{|\Phi_i\rangle\}$ stand for the basis of maximally entangled vectors of two qubits

$$|\Phi_1\rangle \equiv \frac{1}{\sqrt{2}}(|01\rangle + |10\rangle), \quad |\Phi_2\rangle \equiv \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle),$$

$$|\Phi_3\rangle \equiv \frac{1}{\sqrt{2}}(|00\rangle - |11\rangle), \quad |\Phi_4\rangle \equiv \frac{1}{\sqrt{2}}(|01\rangle - |10\rangle). \tag{50}$$

Then H can be alternatively expressed as

$$H = \sum_{i=1}^{4} \lambda_i |\Phi_i\rangle\langle\Phi_i|, \tag{51}$$

where λ_i are decreasingly ordered, real coefficients fulfilling the constraint $\Sigma_i \lambda_i = 0$ (coming from the fact that H has no trace) and

$$\lambda_1 = h_1 + h_2 - h_3, \tag{52}$$

$$\lambda_2 = h_1 - h_2 + h_3, \tag{53}$$

$$\lambda_3 = -h_1 + h_2 + h_3, \tag{54}$$

$$\lambda_4 = -h_1 - h_2 - h_3. \tag{55}$$

The most general simulation protocol using H and LU leads to

$$H' = \sum_k p_k u_k \otimes v_k H u_k^\dagger \otimes v_k^\dagger, \tag{56}$$

where we have assumed, without loss of generality, that H' is also in its canonical form, as in Eqs. (47) and (51), with corresponding coefficients h_i' and λ_i'.

A. Necessary and sufficient conditions for efficient simulation and optimal simulation factor

Let us derive the necessary and sufficient conditions for H to be able to simulate H' using LU and for infinitesimal simulation times. Uhlmann's theorem [18] states that the eigenvalues λ_i' of operator H' in Eq. (56), a unitary mixing of operator H, are majorized by the eigenvalues λ_i of H, that is,

$$\lambda_1' \leqslant \lambda_1,$$

$$\lambda_1' + \lambda_2' \leqslant \lambda_1 + \lambda_2,$$

$$\lambda_1' + \lambda_2' + \lambda_3' \leqslant \lambda_1 + \lambda_2 + \lambda_3,$$

$$\lambda_1' + \lambda_2' + \lambda_3' + \lambda_4' = \lambda_1 + \lambda_2 + \lambda_3 + \lambda_4, \tag{57}$$

where the last equation is trivially fulfilled due to the fact that H and H' are traceless operators. Succinctly, we shall write $\vec{\lambda}' \prec \vec{\lambda}$, as usual [15]. In terms of the coefficients h_i and h_i' the previous conditions read

$$h_1' \leqslant h_1,$$

$$h_1' + h_2' - h_3' \leqslant h_1 + h_2 - h_3,$$

$$h_1' + h_2' + h_3' \leqslant h_1 + h_2 + h_3, \tag{58}$$

and correspond to the s(special)-majorization relation, $\vec{h}' \prec_s \vec{h}$, introduced in Ref. [4]. Thus, we have already recovered the necessary conditions of Ref. [4] for H to be able to *efficiently* simulate H' in LU protocols [19] (and thus, since we are in the two-qubit case, also in LOCC protocols).

In order to see that conditions (57) [and thus conditions (58)] are also sufficient for efficient LU simulation, we concatenate on two other results of majorization theory. The first one (see Theorem II.1.10 of Ref. [15]) states that $\vec{\lambda}' \prec \vec{\lambda}$ if and only if a doubly stochastic matrix m exists such that $\lambda_i' = \Sigma_j m_{ij} \lambda_j$. The second result is known as Birkhoff's theorem [15], and states that the matrix m can always be written as a convex sum of permutation operators $\{P_k\}$, so that

$$\begin{pmatrix} \lambda_1' \\ \lambda_2' \\ \lambda_3' \\ \lambda_4' \end{pmatrix} = \sum_k p_k P_k \begin{pmatrix} \lambda_1 \\ \lambda_2 \\ \lambda_3 \\ \lambda_4 \end{pmatrix}. \tag{59}$$

This means that whenever conditions (57) are fulfilled we can obtain H' from H by using a mixing of unitary operations T_i, where each T_i permutes the vectors $\{|\Phi_i\rangle\}$,

$$H' = \sum_i p_i T_i H T_i^\dagger. \tag{60}$$

Then, all we still need to see is that all $4! = 24$ possible permutations of the vectors $\{|\Phi_i\rangle\}$ can be performed through *local* unitary operations T_i. Recall, however, that any permutation σ, taking elements (1,2,3,4) into $[\sigma(1), \sigma(2), \sigma(3), \sigma(4)]$, can be obtained by composing (several times) the following three transpositions:

$$(1,2,3,4) \rightarrow (2,1,3,4), \tag{61}$$

$$(1,2,3,4) \rightarrow (1,3,2,4), \tag{62}$$

$$(1,2,3,4) \rightarrow (1,2,4,3), \tag{63}$$

where each permutation affects two neighboring elements. The corresponding three basic permutations of $(\Phi_1, \Phi_2, \Phi_3, \Phi_4)$ can be easily obtained using LU. Indeed, in order to permute $(\Phi_1, \Phi_2, \Phi_3, \Phi_4)$ into

$$(\Phi_2, \Phi_1, \Phi_3, \Phi_4),$$

$$(\Phi_1, \Phi_3, \Phi_2, \Phi_4),$$

$$(\Phi_1, \Phi_2, \Phi_4, \Phi_3), \tag{64}$$

we can simply apply, respectively, the following local unitary operations:

$$\frac{I-i\sigma_1}{\sqrt{2}}\otimes\frac{I-i\sigma_1}{\sqrt{2}},$$

$$\frac{I+i\sigma_3}{\sqrt{2}}\otimes\frac{I-i\sigma_3}{\sqrt{2}},$$

$$\frac{I+i\sigma_1}{\sqrt{2}}\otimes\frac{I-i\sigma_1}{\sqrt{2}}. \tag{65}$$

Therefore, any permutation σ of the states (50) can be accomplished through local unitary operations T_i, and any Hamiltonian H' satisfying conditions (58) [equivalently, conditions (57)] can be efficiently simulated with H and LU.

In the following we condense the previous findings into two results, (R1) and (R2), which provide an explicit answer to problems (P1) and (P2), respectively, announced in Sec. II C of the paper. We assume that the two-qubit Hamiltonians H and H' are in their canonical form, with $\vec{\lambda}$, $\vec{h}$, $\vec{\lambda}'$, and $\vec{h'}$ the corresponding vectors of coefficients.

(R1) Hamiltonian H' can be efficiently simulated by H and LOCC—or LU, LU+anc., or LO—if and only if conditions (58) [or, equivalently, conditions (57)] are fulfilled, i.e.,

$$H' \leqslant_{LOCC} H \Leftrightarrow \vec{h}' <_s \vec{h} \Leftrightarrow \vec{\lambda}' < \vec{\lambda}. \tag{66}$$

(R2) The simulation factor $s_{H'|H}$ for LOCC—or LU, LU+anc., or LO—protocols is given by the maximal $s>0$ such that $s\vec{h}' <_s \vec{h}$ or, equivalently, such that $s\vec{\lambda}' < \vec{\lambda}$.

B. Explicit optimal LU protocols

The last question we address is how to actually construct a simulation protocol. That is, given H and H', we show how to simulate sH' using H and LU, for any $s\in[0,s_{H'|H}]$.

A complete answer to this question is given by a probability distribution $\{p_k\}$ and a set of unitary operations $\{u_k\otimes v_k\}$ such that

$$sH' = \sum_k p_k u_k\otimes v_k H u_k^\dagger \otimes v_k^\dagger, \tag{67}$$

where $s\in[0,s_{H'|H}]$, and $s_{H'|H}$ can be obtained using result (R2).

We already argued that it is always possible to choose all $u_k\otimes v_k$ such that they permute the vectors of Eq. (50), so that each $u_k\otimes v_k \equiv T_k$ is just a composition of the local unitary operation of Eqs. (65). As before, let $\{P_k\}_{k=1}^{24}$ denote the 24 permutations implemented by the local unitary operations $\{T_k\}_{k=1}^{24}$. Then the above problem reduces to finding an explicit probability distribution $\{p_k\}$ such that

$$s_{H'|H}H' = \sum_k p_k T_k H T_k^\dagger, \tag{68}$$

or, equivalently, such that

$$s_{H'|H}\vec{\lambda}' = \sum_k p_k P_k \vec{\lambda}. \tag{69}$$

This is done in Appendix B by using standard techniques of convex set theory. There we show how to construct a solution involving at most four terms $p_k T_k$ for $s<s_{H'|H}$, and at most three terms for optimal simulation, that is, when $s=s_{H'|H}$.

VI. CONCLUSIONS

In this paper we have studied Hamiltonian simulation under the broader scope of LOCC protocols. We have focused on infinitesimal-time simulations, for which we have shown that LOCC protocols are equivalent to LU+anc. protocols, also that LU+anc. protocols are in general inequivalent to LU protocols (two-qubit Hamiltonians being an exception). For two-qubit Hamiltonians we have rederived and extended the results of Ref. [4], to finally provide the optimal solution using LOCC.

Thus, the problem of simulating Hamiltonian evolutions has received a complete answer for infinitesimal times and using LOCC, for the simplest case of two-qubit systems. Several interesting questions remain open. On the one hand, the generalization of these results to systems other than two qubits appears challenging. On the other hand, the asymptotic scenario for Hamiltonian simulation, where H is used to simulate H' many times on different systems, certainly deserves a lot of attention.

Finally, we note that entangled ancillary systems have been recently shown to be of interest in nonlocal Hamiltonian simulation [20]. In particular, entanglement can act as a catalyst for simulations, both in the infinitesimal-time and finite-time regimes, in that in the presence of entanglement better time efficiencies can be obtained, although the entanglement is not used up during the simulation but is fully recovered after the manipulations.

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APPENDIX A: EXTREME POINTS OF THE SET NONLOCAL HAMILTONIAN SIMULATIONS ACHIEVABLE BY LU+anc.

In this appendix we show that in LU+anc. simulations any Hamiltonian of the form

$$H' = \langle 0_{A'} 0_{B'} | U \otimes V (H \otimes I_{A'B'}) U^\dagger \otimes V^\dagger | 0_{A'} 0_{B'} \rangle \quad \text{(A1)}$$

can be efficiently simulated by H, for any pair of unitary operations U and V acting on AA' and BB'. The result is valid also for more than two systems after a straightforward generalization of the following proof.

Notice that we can always write U and V using product basis $\{|i_A j_{A'}\rangle\}$ and $\{|i_B j_{B'}\rangle\}$ as

$$U = \sum_{i=0}^{d_A - 1} \sum_{j=0}^{d_{A'} - 1} |i_A j_{A'}\rangle\langle \phi_{ij}|, \quad \text{(A2)}$$

$$V = \sum_{i=0}^{d_B - 1} \sum_{j=0}^{d_{B'} - 1} |i_B j_{B'}\rangle\langle \psi_{ij}|, \quad \text{(A3)}$$

where $\{|\phi_{ij}\rangle\}$ and $\{|\psi_{ij}\rangle\}$ are other orthonormal bases of systems AA' and BB', respectively, and d_κ denotes the dimension of system κ.

To perform this simulation, we need to make the output of the ancilla be the state $|0_{A'} 0_{B'}\rangle$, unentangled with the systems AB. This cannot be achieved by performing just transformations U and V, but by considering also a series of local unitary operations $\{U_a \otimes V_b\}$, $a \in \{0, \cdots, d_{A'} - 1\}$, $b \in \{0, \cdots, d_{B'} - 1\}$,

$$U_a \equiv I \otimes \left(\sum_{l=0}^{d_{A'} - 1} e^{i 2\pi (al/d_{A'})} |l_{A'}\rangle\langle l_{A'}| \right) U, \quad \text{(A4)}$$

$$V_b \equiv I \otimes \left(\sum_{l=0}^{d_{B'} - 1} e^{i 2\pi (bl/d_{B'})} |l_{B'}\rangle\langle l_{B'}| \right) V, \quad \text{(A5)}$$

and a uniform probability distribution $\{p_{ab}\}$, $p_{ab} = 1/(d_{A'} d_{B'})$. Then we have that $U_a^\dagger |0_{A'}\rangle = U^\dagger |0_{A'}\rangle$, and that $\Sigma_a U_a = d_{A'} |0_{A'}\rangle\langle 0_{A'}| U$, and similarly for V_b, so that we obtain

$$\sum_{ab} p_{ab} U_a \otimes V_b (H \otimes I_{A'B'}) U_a^\dagger \otimes V_b^\dagger |0_{A'} 0_{B'}\rangle = |0_{A'} 0_{B'}\rangle\langle 0_{A'} 0_{B'}| U \otimes V (H \otimes I_{A'B'}) U^\dagger \otimes V^\dagger |0_{A'} 0_{B'}\rangle. \quad \text{(A6)}$$

Therefore Eq. (A6) defines a protocol that simulates the Hamiltonian of Eq. (A1) with unit time efficiency.

APPENDIX B: EXPLICIT TWO-QUBIT LU SIMULATION PROTOCOLS

In this appendix we show how to find a probability distribution $\{p_k\}$ and permutations $\{P_k\}$ such that

$$\vec{\mu} = \sum_k p_k P_k \vec{\lambda}, \quad \text{(B1)}$$

for any two given four-dimensional, real vectors $\vec{\lambda}$ and $\vec{\mu}$ ($\vec{\mu} = s\vec{\lambda}'$ in Sec. V B) such that $\vec{\mu} \prec \vec{\lambda}$, where $\Sigma_{i=1}^4 \lambda_i = \Sigma_{i=1}^4 \mu_i = 0$.

We first note two facts that will allow us to use standard techniques of convex set theory: (i) the set $S \equiv \{\vec{\tau} \,|\, \vec{\tau} \prec \vec{\lambda}\}$ is convex, and (ii) $\{P_k \vec{\lambda}\}_{i=1}^{24}$ are the extreme points of S, as it follows from Birkhoff's theorem [15]. We can then proceed as follows.

(a) We check whether $\vec{\mu} = P_i \vec{\lambda}$ for any $i = 1, \ldots, 24$. If we find one such permutation we are done. Otherwise we move to step (b).

(b) Facts (i) and (ii) guarantee that there is at least one permutation P_k, that we call Q_1, and a positive $\epsilon > 0$ such that

$$\vec{\mu} = \epsilon Q_1 \vec{\lambda} + (1 - \epsilon) \vec{\tau}, \quad \text{(B2)}$$

where $\vec{\tau}$ also belongs to S, and therefore satisfies $\vec{\tau} \prec \vec{\lambda}$. In other words, we have to search until we find a permutation Q_1 such that

$$(\vec{\mu} - \epsilon Q_1 \vec{\lambda})/(1 - \epsilon) \prec \vec{\lambda}, \quad \text{(B3)}$$

for some $\epsilon > 0$. Once we have found it we only need to increase ϵ to its maximal value compatible with Eq. (B3). Let q_1 be this maximal value of ϵ. Then we can write

$$\vec{\mu} = q_1 Q_1 \vec{\lambda} + (1 - q_1) \vec{\mu}_2, \quad \text{(B4)}$$

where $\vec{\mu}_2 \prec \vec{\lambda}$ is on one of the surfaces of S—otherwise we could have taken a greater q_1.

Such a surface is, again, a (lower dimensional) convex set, whose extreme points are some of the $P_k \vec{\lambda}$'s, and whose elements $\vec{\tau}$ fulfill $\vec{\tau} \prec \vec{\lambda}$ but with one of the majorization inequalities replaced with an equality. This allows us to repeat points (a) and (b), but now aiming to decompose $\vec{\mu}_2$ as a convex sum of vectors $P_k \vec{\lambda}$. That is, first we check whether $\vec{\mu}_2$ corresponds to $P_k \vec{\lambda}$ for some k. And, if not, we search until we find a permutation P_k, let us call it Q_2, such that, again,

$$(\vec{\mu}_2 - \epsilon Q_2 \vec{\lambda})/(1 - \epsilon) \prec \vec{\lambda}. \quad \text{(B5)}$$

The maximum value of ϵ compatible with this equation, say q, leads to a second term $q_2 Q_2$ [$q_2 = (1 - q_1) q$] for the decomposition of $\vec{\mu}$,

$$\vec{\mu} = (q_1 Q_1 + q_2 Q_2) \vec{\lambda} + (1 - q_1 - q_2) \vec{\mu}_3, \quad \text{(B6)}$$

and to a new $\vec{\mu}_3$ that lies on a surface of yet lower dimensionality of the original convex set S. We iterate the procedure until the remaining vector $\vec{\mu}_l$ lies on a convex surface of S of dimension zero, which means that the surface contains only one element, $\vec{\mu}_l$. In this way we obtain the desired decomposition,

$$\vec{\mu} = \sum_{k=1}^{l} q_k Q_k \vec{\lambda}. \quad \text{(B7)}$$

What is the minimal value of l? For nonoptimal simulation

protocols we have that $\vec{\mu}=s\vec{\lambda}'$, where $s<s_{H'|H}$, and $\vec{\mu}$ is in the interior of S, which is a three-dimensional set. Therefore the above procedure has to be iterated at most three times before we are left with a zero-dimensional surface of S, and the minimal decomposition contains at most $l=4$ terms. For optimal-simulation protocols $\vec{\mu}=s_{H'|H}\vec{\lambda}'$ is already in a surface of S, and therefore the minimal decomposition contains from 1 to 3 terms.

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[11] In this work we assume that local ancillary systems are available at wish in LO protocols (see Sec. III), and thus we make no distinction between LO and LO+anc. (as opposed to Ref. [4]).

[12] In practice, to simulate the *entire* evolution $e^{-it'H'}$ means to fix a division of T' into a (large) number N of regular time intervals of length τ, $T'=N\tau'$, and to have the system, initially in state $|\psi\rangle$, sequentially driven into the state $e^{-ik\tau'H'}|\psi\rangle$, for $k=1,2,\ldots,N$. Perfect dynamics simulation corresponds to taking the large N limit.

[13] Subsequent studies have shown that, in a two-qubit system, $s_{H'|H}$ is often also the minimal time (or *interaction cost*) required to perform the gate $e^{-iH'T'}$ by H' and LU , G. Vidal, K. Hammerer, and J.I. Cirac, Phys. Rev. Lett. **88**, 237902 (2002).

[14] As explained in Ref. [4], local terms such as $I_A\otimes O_B$ can be added and removed by means of local unitary operations, and thus we can safely omit them in the present argumentation.

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[17] One can use the results of Ref. [16], concerning the robustness of entanglement transformations under a perturbation of the state under consideration, to show that the argument of Sec. III B 2 of this paper is also robust under $O(t)$ modifications of a maximally entangled state.

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