Topology identification of autonomous quantum dynamical networks

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Topology identification comprises reconstructing the Hamiltonian, and thus the corresponding interaction terms, by properly processing measurements of its density operator within a fixed time interval. It finds application in several quantum technology contexts, ranging from quantum communication to quantum computing or sensing. In this paper we provide analytical conditions for the solvability of the topology identification problem for autonomous quantum dynamical networks (i.e., as in our case, not explicitly depending on time via the use of an external drive). The solvability condition is then converted in an algorithm for quantum network reconstruction that is easily implementable on standard computer facilities. The obtained algorithm is tested for Hamiltonian reconstruction on numerical examples based on the quantum walks formalism.

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I. INTRODUCTION

A quantum dynamical network is a graph with nontrivial connectivity, composed by quantum-mechanical systems that may exhibit their own time evolution [1]. Studies on quantum networks have several motivations. First of all, there is growing interest in realizing quantum communication backbones, able to connect remote nodes that are linked by quantum channels [2–9]. Secondly, it is worth recalling both the important role of quantum effects in energy transport problems that are popular in many fields of science, such as physics, biology, chemistry, and information science [10–17], as well as relevant applications of quantum networks in many-body physics and quantum computing [18–23].

In all these different contexts, the topology of the networks [24] is a key aspect that highly influences time changes of their state. In fact, time behaviors are determined by the interconnection between the nodes of the network, and this is true for both classical and quantum cases. A meaningful example is provided by the so-called "agreement dynamics" for multiagent systems in network configuration. In such a context, the agreement of all interacting agents in achieving a common objective is reached if and only if the matrix with the agents' interconnections obeys specific properties that depend on the (dynamical) parameters of each agent [25–27]. Another example, more focused on quantum frameworks, is the transport of a quantum particle in a maze, which by construction is a topologically complex network [16]. In such a peculiar case, the interconnection of the maze's constituents defines the efficiency in transferring the particle from the input site to the exit one of the maze in the fastest possible transmission time. It is thus desirable to determine procedures, both analytical and numerical, that allow for the characterization of the geometric properties of a dynamical network constituted by distinct and independent subsystems.

In all cases where network topology is unavailable or uncertain, *topology identification* aims to determine the network structure, and possibly the weights of the links between the nodes of the network, by using measurements of its state evolution [28]. In doing this, we thus assume that the states of the network, or part of them, can be measured.

For networks whose nodes exhibit nonquantum behaviors, several topology identification techniques have been already developed. In this regard, it is worth mentioning techniques based on the dynamic average consensus [29], the inverse covariance estimation method [30], the power spectral analysis [31], compressive sensing [32,33], and also topology reconstruction via a transfer matrix of the network [34], stochastic perturbations [35], or network state matrices using (constrained) Lyapunov equations [36]. Specifically, the latter approach makes use of state measurements of an autonomous linear dynamical network. From such measurements, a Gramian-like matrix is built that enables the reconstruction of the network matrix by solving a Lyapunov equation. On the contrary, in the quantum sciences field, much attention has been devoted to *quantum Hamiltonian reconstruction*, which concerns the issue of determining key elements of the quantum system Hamiltonian from the corresponding equations of motion [37,38]. The main challenge lies in the fact no effective relationship between the Hamiltonian of the system and the state evolution may be present, depending on both the initial state and the value taken by the Hamiltonian parameters. Hence, recently, the problem of quantum Hamiltonian reconstruction has been tackled from a

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different perspective, e.g., by using methods taken from linear systems and control theories [39–41], scalable tomographic reconstruction [42], compressed sensing [43], and gradient-based techniques [44].

In this paper we specifically address the problem of identifying the topology of an autonomous quantum dynamical networks. In the case that a quantum network is regarded as a (single) quantum closed system—whereby, once initialized, it evolves according to its own Hamiltonian—the methods enabling Hamiltonian reconstruction can be successfully employed, and they can be considered as the state of the art for such a task. Instead, if a network structure can be identified, the Hamiltonian is provided by the sum of both the Hamiltonian of each quantum network subsystem and interaction terms, taking into account the coupling between them. Here, the aim of the topology identification is to understand the presence of interaction couplings and their intensity, corresponding one-to-one to the topology of the analyzed network. In this scenario, by starting from the quantum Hamiltonian reconstruction, the following three main results are discussed in this paper. They may be regarded as a generalization to quantum systems of the results in [36]:

(i) We provide sufficient conditions that ensure the solvability of topology identification problems for autonomous quantum networks by measuring the complete state of the network in the time instants within the interval $[0, \tau]$ with $\tau > 0$.

(ii) We propose an algorithm to infer network topology for generic autonomous quantum networks whose state undergoes unitary time evolution. The algorithm is based on the obtained solvability condition and is designed to be implementable on standard computer facilities.

(iii) Sufficient conditions for the solvability of the identification problem are given also in the case of measurements with *partial information*, namely, not containing all the values of the network state at each time instant. Despite that discussions about quantum Hamiltonian reconstruction via measurements of local observables are already present in the literature (e.g., refer to Ref. [45]), we provide analytical results that rely on fulfilling the so-called observability conditions [46] through the partial measurement of the network states in different time instants. In this regard, before proceeding we give a brief definition of observability; the formal definition, indeed, is provided by Eq. (19) in Sec. VI below. Hence, with observability we mean our capability to infer the whole state of a dynamical system, even all its inaccessible components, from measuring it (usually partially) within a finite time interval.

The paper is organized as follows. In Sec. II we introduce the basic mathematical elements that define a dynamical quantum network. In addition, we provide the tools to interpret an arbitrary many-body quantum system as a quantum network. Then, in Sec. III we formulate the topology reconstruction problem by using measurements of the network density operator within the time interval $[0, \tau]$. In Sec. IV we analyze under which analytical conditions the considered topology identification problem, applied to autonomous quantum networks, is solvable by using measurements of the full network density operator within $[0, \tau]$. We prove a theorem that provides a sufficient condition for the solvability of the identification problem by resolving an algebraic commutation relation. Having once determined the conditions for the solvability of the identification problem, in Sec. V we provide an algorithm that can be implemented on standard computer facilities. The analytical results are tested numerically for Hamiltonian reconstruction on a model based on the quantum random walk formalism. In Sec. VI we give preliminary results on topology identification when the network state is only partially measured. Specifically, we show that it is possible to reconstruct the Hamiltonian of an autonomous quantum network if the latter is observable, and we can measure the diagonal elements of its density operator by initializing the network on linearly independent initial states in different runs. Finally, a discussion of the results and some outlooks (Sec. VII) concludes the paper.

II. DYNAMICAL QUANTUM NETWORKS

Let us introduce a dynamical quantum network as a quantum system with total dimension d that is the collection of quantum subsystems. According to the laws of quantum mechanics, if the quantum system is an isolated system, then the time evolution of its state is described by a *unitary* transformation. Thus its state vector $|\psi_t\rangle \equiv \boldsymbol{\psi}_t = (\psi_1, \ldots, \psi_d)^T \in \mathbb{C}^d$ is propagated over time by the linear *unitary* operator $\mathcal{U}$ such that

$$\boldsymbol{\psi}_t = \mathcal{U}_{t,0}\, \boldsymbol{\psi}_0 \tag{1}$$

with $\boldsymbol{\psi}_0 = \boldsymbol{\psi}_{t_0}$. Along with the state vector $\boldsymbol{\psi}_t$, we can also introduce the density operator (denoted as ρ_t) of the network. It is defined by the outer product of $\boldsymbol{\psi}_t$, i.e., $\rho_t \equiv \boldsymbol{\psi}_t \boldsymbol{\psi}_t^\dagger$ where $(\cdot)^\dagger$ stands for the conjugate transpose (or Hermitian transpose) of the operator $(\cdot)$. The density operator provides the statistical description of the state of any quantum system, thereby, in the specific case of a quantum network, returning both the quantum description of each network subsystem and all the interference patterns (and thus nonzero quantum correlations) between them. In this regard, it is worth noting that the latter originates only if the nodes of the network are interacting subsystems. As known from quantum mechanics principles [47,48], at any time instant t the density operator ρ_t must obey the following constraints: ρ_t is (i) an Hermitian operator, namely, $\rho_t^\dagger = \rho_t$; (ii) positive semidefinite, i.e., given a generic quantum state $\boldsymbol{\phi}$, $\boldsymbol{\phi}^\dagger \rho_t\, \boldsymbol{\phi} = |\boldsymbol{\phi}^\dagger \boldsymbol{\psi}_t|^2 \geqslant 0$; and (iii) is trace preserving, i.e., $\mathrm{Tr}[\rho_t] = 1$. Among the consequences, this implies that the elements along the diagonal of ρ_t are always real numbers summing to 1. Moreover, the time evolution of the density operator follows the so-called Liouville–von Neumann equation for any $t \in [0, \infty)$, i.e.,

$$\dot{\rho}_t = \frac{d}{dt}\rho_t = -\frac{i}{\hbar}[H, \rho_t], \tag{2}$$

that returns the solution $\rho_t = \mathcal{U}_{t,0}\rho_0 \mathcal{U}_{t,0}^\dagger$. In Eq. (2), H is the Hamiltonian of the network, $[K, J]$ denotes the commutator between the operators K and J: $[K, J] = KJ - JK$, and $\hbar$ is the reduced Planck constant. By means of Eq. (2), one is able to propagate (over time) the initial state ρ_0 ensuring that all its properties (i)–(iii) are automatically fulfilled. By solving Eq. (2) as a function of $\boldsymbol{\psi}_t$, the Schrödinger equation $i\hbar\, \dot{\boldsymbol{\psi}}_t = H\boldsymbol{\psi}_t$ is recovered, as well as Eq. (1).

Remark 1. Instead of solving the Liouville–von Neumann equation (2) to get the quantum network dynamics, it may useful to work with the column vector $\boldsymbol{\lambda}_t$, which is obtained by vectorizing the density operator ρ_t:

$$\begin{aligned}\boldsymbol{\lambda}_t &\equiv \mathrm{vec}[\rho_t] \\ &= \left(\rho_t^{(11)}, \ldots, \rho_t^{(d1)}, \rho_t^{(12)}, \ldots, \rho_t^{(d2)}, \ldots, \rho_t^{(dd)}\right)^T \in \mathbb{C}^{d^2\times 1}.\end{aligned} \tag{3}$$

In this way, according to the superoperator formalism [49], the Liouville–von Neumann equation (2) can be written as a linear differential equation in the column vector $\boldsymbol{\lambda}_t$:

$$\dot{\boldsymbol{\lambda}}_t = \mathcal{L}\,\boldsymbol{\lambda}_t \quad \text{namely} \quad \boldsymbol{\lambda}_t = e^{\mathcal{L}(t-t_0)}\boldsymbol{\lambda}_0, \tag{4}$$

where $\mathcal{L} = -\frac{i}{\hbar}(\mathbb{I}_d \otimes H - H^T \otimes \mathbb{I}_d) \equiv -\frac{i}{\hbar}\widetilde{H} \in \mathbb{C}^{d^2\times d^2}$, $\mathbb{I}_d$ is the identity matrix of size d, and $\otimes$ denotes the Kronecker product. By construction, $\mathcal{L}$ is a skew-Hermitian (or anti-Hermitian) operator, meaning that $\mathcal{L}^\dagger + \mathcal{L} = 0$.

The linear formulation of quantum network dynamics will be adopted in Sec. VI, where we will address the solvability of topology identification problems with partial information.

Quantum networks from many-body systems

For practical applications in quantum communication and computing, a quantum network is usually constituted by N interacting ℓ-level quantum systems, corresponding to a node of the quantum network. Thus, in this section we briefly discuss how one can deal with the coupling structure of a many-body system composed of interacting subsystems and then express the time evolution of the corresponding density operator via an instance of the Liouville–von Neumann equation (2). In this way, the identification of the unknown interaction structure of a quantum many-body system can be achieved by addressing the reconstruction of the Hamiltonian in (2), as we have formulated below.

Under the hypothesis that a quantum network is provided by N ℓ-level quantum systems, the dimension of the network is equal to $d = \ell^N$, and, concerning the network Hamiltonian, the contributions associated to each node of the network can be decoupled by those of the coupling terms. Formally,

$$H = H_0 + H_{\mathrm{int}} = \sum_{k=1}^{N} \omega_k H_k + H_{\mathrm{int}}, \tag{5}$$

where k is the index over the network nodes. It is worth noting that a different characteristic frequency ω_k and a local Hamiltonian H_k is associated to each node, while H_{int} denotes the interaction Hamiltonian. All the operators H_k, for $k = 1, \ldots, N$, and H_{int}, are Hermitian with size d.

In the quantum many-body systems scenario, it is common practice to assume two-body interactions and compositions of them at any instant of time t. This means that the interaction Hamiltonian H_{int} can be further decomposed in a sum of $D \equiv N^2 - N = N(N-1)$ coupling terms A_kA_j, with $k \neq j$, each of them corresponding to one specific link. In this regard, it is worth noting that A_kA_j is the shorthand notation for the tensor product of A_k and A_j. Instead, A_k denotes the operator that is associated to the kth node of the network and is responsible for the interaction with the jth node through the coupling A_kA_j. This means that

$$H_{\mathrm{int}} = \sum_{k,j=1;k\neq j}^{N} \alpha_{k,j} A_k A_j. \tag{6}$$

Hence, by substituting (6) in (5), it holds that the Liouville–von Neumann equation of a quantum many-body system (written as a dynamical network) is given by

$$\dot{\rho}_t = -\frac{i}{\hbar}[(H_0 + \boldsymbol{\alpha}^T C\boldsymbol{\alpha}), \rho_t] = R_0(t) - \frac{i}{\hbar}[\boldsymbol{\alpha}^T C\boldsymbol{\alpha}, \rho_t], \tag{7}$$

where $R_0(t) \equiv -i[H_0, \rho_t]/\hbar$ is known and completely determined by the knowledge of the local dynamics of the network, while $\boldsymbol{\alpha}$ and C are provided by the relations

$$\begin{aligned}\boldsymbol{\alpha} &= (\sqrt{\alpha_{1,2}}\,\mathbb{I}_d, \ldots, \sqrt{\alpha_{N,N-1}}\,\mathbb{I}_d)^T \in \mathbb{C}^{Dd\times d} \\ C &= \mathrm{diag}(\{A_kA_j\}) \in \mathbb{C}^{D(d\times d)}.\end{aligned}$$

Further details can be found in Appendix A, where we also provide a microscopic derivation of a quantum network by using the many-body formalism and writing each operator A_k, $k = 1, \ldots, N$, as a function of a complete orthonormal basis of eigenoperators.

Remark 2. The complete structure of the operator C (sparse Hermitian matrix) is defined by the laws of quantum mechanics ruling two-body interactions. This means that the only unknown quantity to be reconstructed, returning the topology of the network, is the vector $\boldsymbol{\alpha}$ that contains all the interaction couplings.

III. PROBLEM FORMULATION

Consider a quantum dynamical network whose state evolution over time is described by the Liouville–von Neumann equation (2). We assume that (i) the system Hamiltonian H is not directly available, and (ii) the density operator ρ_t or a portion of it is measured during the time interval $[0, \tau]$.

In the following we will address the problem of identifying the topology of a generic autonomous quantum dynamical network by mainly following the prescription of *network reconstruction* problems as given in the engineering literature. Specifically, the network reconstruction problem involves the identification of the exact value of the Hamiltonian H of the quantum network (it corresponds to infer the vector $\boldsymbol{\alpha}$ of interaction couplings if one has knowledge of the quantum many-body structure) on the basis of measurements of (part of) the density operator ρ_t or equivalently, of the ensemble vector $\boldsymbol{\lambda}_t$.

We will provide analytical conditions under which this important prerequisite holds, and we will present an algorithm for the Hamiltonian reconstruction problem.

IV. TOPOLOGY IDENTIFICATION WITH FULL INFORMATION

In this section we provide analytical conditions that ensure the solvability of the topology identification problem for autonomous quantum networks by measuring the full density operator ρ_t within the time interval $[0, \tau]$. For this purpose, let us consider the density operator ρ_t for any $t \in [0, \tau]$ and take the network Hamiltonian H as a d-dimensional Hermitian

operator $\in \mathbb{C}^{d\times d}$. Moreover, we also assume that H has zero diagonal entries. Any matrix M with these two properties (i.e., Hermitianity and zero diagonal entries) is here denoted as *admissible*, and the set of all admissible matrices as

$$\mathcal{A} \equiv \{M \in \mathbb{C}^{d\times d} \mid M = M^\dagger \text{ and } M_{ii} = 0, \ \ \forall i = 1, \ldots, d\}. \tag{8}$$

By solving Eq. (2), we get a specific trajectory ρ_t with $t \in [0, \tau]$, for any given initial state ρ_0. Thus the set of admissible matrices that allows for such data is given by

$$\mathcal{A}_\rho \equiv \left\{M \in \mathcal{A} \mid \dot{\rho}_t = -\frac{i}{\hbar}[M, \rho_t] \ \forall t \in [0, \tau]\right\}. \tag{9}$$

In addition, let us define the solvability condition of the topology identification problem:

Definition 1. Let ρ_t be given for $t \in [0, \tau]$. Then the topology identification problem is called *solvable* if $\mathcal{A}_\rho = \{H\}$.

Now, by integrating Eq. (2) and taking the network Hamiltonian as an admissible operator, we provide a *sufficient condition* for the solvability of the aforementioned identification problem in the form of the following theorem.

Theorem 1. Define the matrices

$$P \equiv \int_0^\tau \rho_t \, dt \tag{10}$$

$$Q \equiv i\hbar\,(\rho_\tau - \rho_0), \tag{11}$$

with $\tau > 0$ arbitrary. Then the topology identification problem is solvable if there exists a **unique** admissible $\hat{M} \in \mathcal{A}$ that satisfies the relation

$$[\hat{M}, P] = Q. \tag{12}$$

The proof of Theorem 1 is in Appendix B. As it will be shown later, for a given choice of ρ_0 and τ, the knowledge of the density operator ρ_t in a set of time instants $t \in [0, \tau]$, whose number increases at least linearly with the number d of quantum network's nodes, may be sufficient to solve the topology identification problem. However, the larger the number of time instants at which ρ_t is evaluated (for a fixed value of τ) the smaller the topology reconstruction error.

Remark 3. For the purpose of topology identification, let us observe once more that taking a quantum many-body system as the quantum network is an instance of the more general problem that we have previously formulated. In fact, by integrating Eq. (7) within $[0, \tau]$ and defining the matrices $P \equiv \int_0^\tau \rho_t \, dt$ and

$$Q \equiv i\hbar\,(\rho_\tau - \rho_0) - [H_0, P],$$

the problem of identifying the interaction Hamiltonian $H_{\text{int}} = \boldsymbol{\alpha}^T C \boldsymbol{\alpha}$ is again solvable if there exists a **unique** admissible $\hat{M} \in \mathcal{A}$ that satisfies $[\hat{M}, P] = Q$.

In Theorem 1 the matrices P and Q can be computed from data. Thus, in terms of topology identification, we conclude that solving Eq. (12) for $\hat{M} \in \mathcal{A}$ leads to an effective method to reconstruct H from measurements of ρ_t for $t \in [0, \tau]$. However, one also needs to address the issue of determining under which conditions there exists a **unique** solution $\hat{M} \in \mathcal{A}$ to Eq. (12). In this regard, a *necessary and sufficient condition* for the uniqueness of $\hat{M} \in \mathcal{A}$ is provided by the following proposition, whose proof is in Appendix C.

Proposition 1. There exists a unique $\hat{M} \in \mathcal{A}$ satisfying (12) *if and only if* the zero matrix (operator with all terms equal to zero and denoted as $\emptyset$) is the only element of $\mathcal{A}$ that commutes with P.

We can associate a corollary to Proposition 1: *A necessary condition for the uniqueness of the nonzero solution $\hat{M} \in \mathcal{A}$, resulting by solving the equation $MP - PM = Q$, is that $\hat{M}$ does not commute with P.* This corollary is a direct consequence of Proposition 1 and can be used as a preliminary check to evaluate whether the solution $\hat{M} \neq 0$ of the topology identification problem may be effectively unique. In fact, if $[\hat{M}, P] = 0$, then $\hat{M}$ is definitely not unique. Moreover, if $Q \neq \emptyset$, then from Proposition 1, the existence of a unique admissible solution $\hat{M} \neq \emptyset$ that solves the equation $MP - PM = Q$ with P and Q computed from data is guaranteed. From these theoretical results, we can put in place an effective strategy to solve the topology identification problem here considered. This strategy relies in measuring the density operator ρ_t of the network within the time interval $[0, \tau]$ until the equation $MP - PM = Q$ has a nonzero solution $\hat{M} \in \mathcal{A}$ that does not commute with P. A reconstruction algorithm will thus be presented in the next section.

V. AN ALGORITHM FOR QUANTUM NETWORK RECONSTRUCTION

In this section we provide an algorithm for the reconstruction of the quantum network Hamiltonian that requires, as input data, measurements of all the elements of ρ_t. In this regard, let us recall that: (i) the reconstruction problem is solvable *if* there exists a unique matrix $\hat{M} \in \mathcal{A}$ that satisfies the relation $[\hat{M}, P] = Q$ with P, Q computed from measured data (Theorem 1); (ii) there exists a unique $\hat{M} \in \mathcal{A}$ obeying $[\hat{M}, P] = Q$ *if and only if* the zero matrix $\emptyset$ is the only element of $\mathcal{A}$ that commutes with P (Proposition 1). Conditions (i) and (ii) are the guidelines to formulate the reconstruction algorithm. Theorem 1 and Proposition 1 imply that if the reconstruction of the network Hamiltonian (here we are interested only in the interaction components, i.e., the network topology) is solvable, then the solution to this problem can be obtained by determining the unique Hermitian operator with zero diagonal elements that obey Eq. (12).

One way to resolve the matrix equation $[M, P] = Q$, under the constraint of the M Hermitian operator, is to vectorize the matrix equation by writing a standard system of *linear* equations and then imposing the Hermitian symmetry of M by means of *linear* constraints. Specifically, by defining the operator

$$\widetilde{P} \equiv (P^T \otimes \mathbb{I}_d - \mathbb{I}_d \otimes P) \in \mathbb{C}^{d^2\times d^2} \tag{13}$$

and reshaping the matrices M and Q in column vectors of dimension d^2, denoted, respectively, as $\boldsymbol{m} \equiv \text{vec}[M]$ and $\boldsymbol{q} \equiv \text{vec}[Q]$, the matrix equation $[M, P] = Q$ can be recast in the linear equation

$$\widetilde{P}\boldsymbol{m} = \boldsymbol{q}. \tag{14}$$

Then, instead of resolving the equation $\widetilde{P}\boldsymbol{m} = \boldsymbol{q}$ as a function of $\boldsymbol{m}$ with the constraint that the resulting solution satisfies the property of Hermitian symmetry, we write an *enlarged* linear

system such that the required constraints (Hermitian symmetry and solution with diagonal elements equal to zero) are automatically fulfilled. For this purpose, we define the matrices $F_1 \in \mathbb{R}^{d\times d^2}$ and $F_2 \in \mathbb{C}^{\frac{d(d-1)}{2}\times d^2}$. The former has almost all terms equal to zero, except to the $(k+1, kd+1)$-th elements, with $k = 0, \ldots, d-1$, that are all equal to 1. This guarantees that, by imposing $F_1\boldsymbol{m} = \emptyset$, all the diagonal elements of M (corresponding to the $(kd+1, kd+1)$-th diagonal elements of M with $k = 0, \ldots, d-1$), are equal to zero. Instead, F_2 is designed to ensure that $M = M^\dagger$. For the sake of a clearer presentation, here we provide a simplified expression of F_2 under the hypothesis that M is a matrix with real elements. In such a case, one can easily check that the validity of the relation $F_2\boldsymbol{m} = \emptyset$ is equivalent to ensure that $M = M^T$, where

$$F_{2,kj} \equiv \begin{cases} +1, & \text{if } \ j = (\ell-1)d + i \\ -1, & \text{if } \ j = (i-1)d + \ell \\ 0, & \text{otherwise,} \end{cases}$$

with $k = 1, \ldots, d(d-1)/2$, $\ell = 1, \ldots, d-1$, and $i = \ell + 1, \ldots, d$. A similar, though more involved, expression holds in case M is a matrix of complex numbers. In conclusion, the enlarged linear system that recasts the matrix equation $[M, P] = Q$, with M Hermitian and diagonal elements equal to zero, is given by

$$\widetilde{P}'\boldsymbol{m} = \boldsymbol{q}' \quad \text{where} \quad \widetilde{P}' \equiv \begin{bmatrix} \widetilde{P} \\ F_1 \\ F_2 \end{bmatrix} \quad \text{and} \quad \boldsymbol{q}' \equiv \begin{bmatrix} \boldsymbol{q} \\ \emptyset \\ \emptyset \end{bmatrix}. \tag{15}$$

Accordingly, the algorithm for the reconstruction of the quantum network Hamiltonian, using measurements of the whole density operator ρ_t, is defined as follows.

Algorithm 1. Network Hamiltonian reconstruction with full information:

If $\text{rank}\,(\widetilde{P}') = d^2 \implies \hat{\boldsymbol{m}} = (\widetilde{P}')^+\boldsymbol{q}'$;

otherwise, $[M, P] = Q$ has nonunique solutions $\hat{M} \in \mathcal{A}_\rho$.

$(\widetilde{P}')^+ \equiv \widetilde{P}'^*(\widetilde{P}'\widetilde{P}'^*)^{-1}$ denotes the Moore-Penrose right inverse of $\widetilde{P}'$, with $\widetilde{P}'^*$ the corresponding conjugate transpose. Then $\hat{M}$ is obtained by applying the inverse of the vectorization operation, thus reshaping the column vector $\hat{\boldsymbol{m}}$ in a square Hermitian operator with diagonal elements equal to zero.

It is worth observing that asking for $\text{rank}(\widetilde{P}') = d^2$ is the necessary requirement for the uniqueness of the solution $\hat{M} \in \mathcal{A}_\rho$ solving the matrix equation $[M, P] = Q$. However, this does not imply that a value of $\hat{\boldsymbol{m}} = (\widetilde{P}')^+\boldsymbol{q}'$ cannot be obtained from the calculation, albeit in this stage we do not have control of the magnitude of the reconstruction error. Moreover, Algorithm 1 has the advantage of determining its solution by solving a system of linear equations (i.e., $\widetilde{P}'\boldsymbol{m} = \boldsymbol{q}'$) that can be achieved using efficient computational tools.

Case study: Quantum random walk model

As a case study of network Hamiltonian reconstruction, let us consider the quantum random walk model [50,51] that is the transposition of the concept of classical random walk to the quantum context. Specifically, we take into account a single walker moving on a graph G. The latter is described by the pair $G = (\mathcal{N}, \mathcal{E})$, where $\mathcal{N}$ denotes the set of nodes (or vertices) of the graph and $\mathcal{E}$ is the set of links that couple pairs of nodes $(\mathcal{N}_k, \mathcal{N}_\ell)$. Each node is associated to a different walker position, while the links correspond to the probability that the walker jumps from one node to another. The links belonging to $\mathcal{E}$ can be summarized in the adjacency matrix A, whose elements are given by

$$A_{kj} = \begin{cases} 1, & \text{if } \ (\mathcal{N}_k, \mathcal{N}_j) \in \mathcal{E} \\ 0, & \text{if } \ (\mathcal{N}_k, \mathcal{N}_j) \neq \mathcal{E}. \end{cases}$$

Note that here we are implicitly assuming that the links are equally weighted with weights all equal to 1. Moreover, if all the positions of the walker are states with the same energy, then one is allowed to set such energy to a reference constant value. Usually the reference energy value is taken equal to zero, with the result that the Hamiltonian H of the quantum walker is identically equal to the adjacency matrix A ($H = A$).

Also, the state of the quantum walker, moving on the graph G with d nodes, is provided by a density operator $\rho_t \in \mathbb{C}^{d\times d}$. The diagonal elements of ρ_t define the probabilities that the walker is in each of the allowed positions (such terms are denoted as *populations*), while the off-diagonal elements are the so-called *quantum coherence* terms that identify interference patterns between nodes. The initial state ρ_0 is taken with all the coherence terms equal to 0 and only one population equal to 1 (randomly chosen in each realization of the network dynamics).

By addressing the topology identification problem with full information, we measure the elements of the density operator ρ_t within the time interval $t \in [0, \tau]$, and the reconstruction problem consists in determining the exact value of the elements of the adjacency matrix A, i.e., in identifying the presence of a link between the nodes of the graph. To validate the performance of Algorithm 1, we numerically solve the time evolution of the state for 100 random networks A, each of them with an increasing number $d \in [2, 30]$ of nodes. The network dynamics is computed with resolution (sampling period) $\delta t = 10^{-2}$. This entails that the total number of samples that compose the quantum network evolution is equal to the ratio $n_s = \tau/\delta t = \tau/10^{-2}$. The random networks are sampled by an Erdős-Rényi distribution, whereby the nodes of the network are randomly connected and each link is included in the graph with probability p_{link} [52,53]. We recall that, according to this model, a network with d nodes and m links is sampled with probability

$$p_{\text{graph}} = p_{\text{link}}^m (1 - p_{\text{link}})^{\binom{d}{2}-m},$$

where $\binom{n_1}{n_2} \equiv \frac{n_1!}{n_2!(n_1-n_2)!}$ is the binomial coefficient and $2^{\binom{d}{2}}$ the total number of networks with d nodes. Instead, regarding the initialization, each time the initial density operator of the network is randomly chosen among one of the states $\rho_0 = \boldsymbol{e}_k\boldsymbol{e}_k^T$ with $k = 1, \ldots, d$ (thus with just one node excited). This choice is the simplest to be realized experimentally. The evolution of the network is then evaluated at discrete time instants within the time interval $[0, \tau]$, where τ is equal to 1, 2, or 3, all expressed in natural units such that $\hbar$ can be set to 1. In our simulations the operator P (it is provided by the

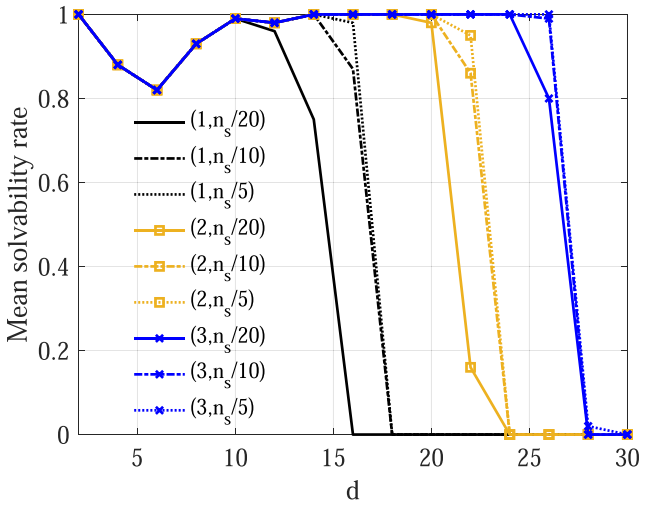

FIG. 1. Plot of the mean solvability rate $\bar{\mathfrak{s}}$ as a function of $d \in [2, 30]$ (number of nodes) and of the pairs $(\tau, \widetilde{n}_s)$, with $\tau \in \{1, 2, 3\}$ and $\widetilde{n}_s \in \{n_s/20, n_s/10, n_s/5\}$. Specifically, for the considered values of d and $p_{\text{link}} = 0.5$, the topology identification problem is solved for 100 random Erdős-Rényi quantum networks. The black, orange, and blue curves refer, respectively, to $\tau = 1, 2, 3$.

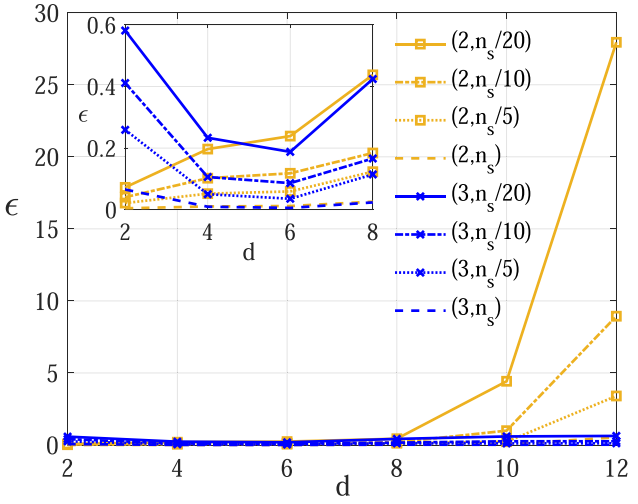

FIG. 2. Plot of the relative reconstruction error ϵ in identifying single random Erdős-Rényi quantum networks with $p_{\text{link}} = 0.5$. The relative error ϵ is plotted as a function of $d \in [2, 12]$ for different pairs $(\tau, \widetilde{n}_s)$, with $\tau \in \{1, 2\}$ and $\widetilde{n}_s \in \{n_s/20, n_s/10, n_s/5, n_s\}$. In the figure, the red and blue curves respectively refer to $\tau = 2, 3$.

integral of ρ_t) within the interval $[0, \tau]$ is approximated as

$$P \equiv \int_0^\tau \rho_t \, dt \approx \sum_{k=1}^{\widetilde{n}_s} \int_{t_{k-1}}^{t_k} \rho_t \, dt$$

$$\approx \frac{1}{2} \sum_{k=1}^{\widetilde{n}_s} (t_k - t_{k-1}) \left(\rho_{t_{k-1}} + \rho_{t_k} \right). \tag{16}$$

Numerically, the integral $\int_0^\tau \rho_t \, dt$ is computed by assigning different values to $\widetilde{n}_s$, i.e., $n_s/20$, $n_s/10$, $n_s/5$, and n_s, with the aim to evaluate how the reconstruction performance of Algorithm 1 depends on the resolution used to monitor the network dynamical evolution. Note that the smaller the value of $\widetilde{n}_s$, the fewer evaluations of ρ_t are required. Moreover, for each realization of the simulated dynamics, we introduce a label $\mathfrak{s}$, denoted as *solvability label*, that takes two values: one if the quantum network reconstruction problem is solvable [i.e., $\hat{\boldsymbol{m}} = (\widetilde{P}')^{+} \boldsymbol{q}'$ for $\text{rank}(\widetilde{P}') = d^2$] with P approximated as in Eq. (16), and zero otherwise, in agreement with the prescriptions of Algorithm 1.

In Fig. 1 we plot the mean solvability rate $\bar{\mathfrak{s}}$ in identifying the topology of random Erdős-Rényi quantum networks as a function of $d \in [2, 30]$. The mean solvability rate is equal to the arithmetic mean of $\mathfrak{s}$ obtained in each of the 100 network reconstructions for every chosen set of parameters, namely,

$$\bar{\mathfrak{s}} \equiv \frac{1}{100} \sum_{q=1}^{100} \mathfrak{s}_q. \tag{17}$$

The value of $\bar{\mathfrak{s}}$ is plotted as a function of both the duration τ and the number of samples $\widetilde{n}_s$ used to calculate numerically the operator P. From Fig. 1 the following numerical evidences can be observed: (i) By increasing the number of nodes, a linearly larger value of τ is required to successfully carry out the network Hamiltonian reconstruction problem. This means that to reconstruct the topology of an Erdős-Rényi quantum network, we need to monitor the time evolution of its state, at least for a linearly longer period of time, independently of the value of p_{link}. As an example, for the simulations in Fig. 1 where the value of τ is fixed and taken equal to 1,2,3 (corresponding, respectively, to the back, orange, and blue curves in the figure), the mean solvability rate $\bar{\mathfrak{s}} = 0 \; \forall d > d_c$, with d_c the critical number of nodes depending on τ. For the blue curves, e.g., $d_c = 28$; however, one can recover $\bar{\mathfrak{s}} = 1$ (and thus, high-probability topology reconstruction) for $d > d_c$ if the value of τ were increased, linearly with the number of nodes. Moreover, notice that for quantum networks with few nodes, $\bar{\mathfrak{s}}$ may be smaller than the maximum value 1 that instead is reached for a larger number of nodes up to the critical value d_c. For small values of d, $\bar{\mathfrak{s}} \neq 1$ since the trajectories of the network dynamics in such case are oscillating. Thus repeated evaluations of the latter at regular discrete times, as in our simulations, provide similar results and thus may not be so informative. In conclusion, $\bar{\mathfrak{s}} \neq 1$ can be considered as a *finite-size* effect; in fact, by increasing the dimension of the network, such effect is lost until Algorithm 1 loses its effectiveness due to the finite and fixed value of τ. (ii) The mean solvability rate $\bar{\mathfrak{s}}$ practically does not depend on the number of samples $\widetilde{n}_s$ used to derive P. Hence, the identification problem is solvable also by computing the operator P by means of few measurements of ρ_t within $[0, \tau]$. However, one could expect that by decreasing the number of measured values of ρ_t (needed for the computation of P), the reconstruction error dramatically increases. This is what has been quantified in Fig. 2, where in case the quantum network reconstruction problems are solvable, we plot the relative reconstruction error ϵ in identifying single random Erdős-Rényi quantum networks by using full information. The relative reconstruction error is defined as

$$\epsilon \equiv \frac{\|\hat{M} - A\|_2}{\|A\|_2}, \tag{18}$$

where $\|\cdot\|$ denotes the L^2 operator norm, A is the network adjacency matrix (Hamiltonian) to be identified, and $\hat{M} \in \mathcal{A}_\rho$ is the reconstructed one returned by Algorithm 1. In Fig. 2 the relative error ϵ is plotted as a function of the number of nodes and for eight different pairs $(\tau, \widetilde{n}_s)$, with $\tau \in \{1, 2\}$ and $\widetilde{n}_s \in \{n_s/20, n_s/10, n_s/5, n_s\}$. As one can observe (also from the inset), the relative reconstruction error is only slightly greater than 0 for $d \leqslant 8$, independently of the value of τ and $\widetilde{n}_s$. Of course, also in this case, ϵ is larger if $\widetilde{n}_s = n_s/20$, i.e., if only few values of the network density operator are taken into account. Instead, the larger values of ϵ are observed in Fig. 2 for $d > 8$, where the relative reconstruction error remains small for $\tau = 3$ and $(\tau = 2, \widetilde{n}_s = n_s)$. This means that, despite that the identification problem is solvable, the reconstruction error can dramatically increase, especially by decreasing the value of τ and using few measurement outcomes to compute P.

VI. SOLVABILITY OF TOPOLOGY IDENTIFICATION WITH PARTIAL INFORMATION

In this section we give some preliminary results for the situation where the whole network state is not available for measurements. Specifically, we address the solvability of topology identification problems for autonomous quantum dynamic networks by using measurements of only the *diagonal entries* of ρ_t, the solution of the Liouville–von Neumann equation (2). Measuring all the elements of ρ_t, indeed, is just a *sufficient condition* to successfully reconstruct the topology of a quantum network in the single realization of its dynamics for a generic initial state ρ_0. This means that by collecting data on ρ_t, the reconstruction problem can be solvable also in the case that only a portion of ρ_t is measured.

As stressed in Remark 1, the Liouville–von Neumann equation can be written as a linear differential equation of the state vector $\boldsymbol{\lambda}_t \in \mathbb{C}^{d^2\times 1}$ by means of the vectorization of ρ_t. In this way one gets $\dot{\boldsymbol{\lambda}}_t = \mathcal{L}\boldsymbol{\lambda}_t$, with $\mathcal{L}$ the skew-Hermitian operator. For our purposes, let us associate to the dynamical equation $\dot{\boldsymbol{\lambda}}_t = \mathcal{L}\boldsymbol{\lambda}_t$ an *output equation* that selects only the diagonal elements of ρ_t at each time t. The output equation is

$$\boldsymbol{y}_t = C\boldsymbol{\lambda}_t \in \mathbb{C}^{d\times 1},$$

with $C \in \mathbb{R}^{d\times d^2}$ defined as

$$C_{kj} = \begin{cases} 1, & \text{if } \ j = (k-1)d + k \\ 0, & \text{otherwise,} \end{cases}$$

where d is the dimension of the quantum network. It is worth noting that the dynamical and output equations are fully characterized by the initial state $\boldsymbol{\lambda}_0$ and the pair $(C, \mathcal{L})$. In what follows we will resort to the concept of *observability* [46]. The pair $(C, \mathcal{L})$ is observable if

$$\operatorname{rank}\begin{bmatrix} C \\ C\mathcal{L} \\ \vdots \\ C\mathcal{L}^{d^2-1} \end{bmatrix} = d^2. \tag{19}$$

For the sake of clarity, the output trajectory $\boldsymbol{y}_t$ in the time interval $[0, \tau]$, resulting from the initial state $\boldsymbol{\lambda}_0$, is denoted as $\boldsymbol{y}_{\lambda_0}(t)$.

Under the assumption that the quantum network is observable, we provide (in the following Proposition) a condition under which the operator $\mathcal{L}$ can be *uniquely* identified from *multiple* partial measurements of ρ_t with C fixed *a priori*.

Proposition 2. Let $\boldsymbol{\lambda}_0^{(\ell)}$ be d^2 linearly independent initial states for $\ell = 1, \ldots, d^2$. Let us also assume to measure the output equation $\boldsymbol{y}_t$ that is obtained by initializing the quantum network in each of the d^2 input states, thus having access to $\boldsymbol{y}_{\lambda_0^{(\ell)}}(t)$ for $t \in [0, \tau_\ell]$, $\tau_\ell > 0$ and $\ell = 1, \ldots, d^2$. If the pair $(C, \mathcal{L})$ is observable, then the operator $\mathcal{L}$ is **uniquely** identifiable from $[\boldsymbol{y}_{\lambda_0}^{(1)}, \ldots, \boldsymbol{y}_{\lambda_0}^{(d^2)}]$. In other words, $\overline{\mathcal{L}} = \mathcal{L}$ for any pair $(C, \overline{\mathcal{L}})$ that generates the outputs $[\boldsymbol{y}_{\lambda_0}^{(1)}, \ldots, \boldsymbol{y}_{\lambda_0}^{(d^2)}]$.

The proof of Proposition 2 is in Appendix D. We observe that the only assumptions needed to prove Proposition 2 are (i) the observability of the pair $(C, \mathcal{L})$ and (ii) the generation of d^2 linearly independent input vectors $\boldsymbol{\lambda}_0^{(\ell)}$, with $\ell = 1, \ldots, d^2$. Instead, it does not matter whether the operator $\mathcal{L}$ obeys specific symmetry properties. We can thus conclude that in the case of partial information on the density operator of the network, we need to repeat d^2 times the dynamical evolution of the quantum network by starting from d^2 independent initial conditions $\boldsymbol{\lambda}_0$, each of them corresponding to a specific initial state $\rho_0 \equiv |\psi_0\rangle\langle\psi_0| \in \mathbb{C}^{d\times d}$. A quite trivial choice could be to take ρ_0 equal to $|k\rangle\langle j| \equiv \boldsymbol{e}_k\boldsymbol{e}_j^T$ for $k, j = 1, 2, \ldots, d$, where $\boldsymbol{e}_k$ denotes the kth standard $\mathbb{R}^d$ basis vector. However, let us note that the operators $|k\rangle\langle j|$, with $k \neq j$, are not Hermitian and do not have unit trace. Thus, these states are not physical, in the sense that they cannot be experimentally prepared. To overcome this issue one can decompose $|k\rangle\langle j|$ as a function of the fixed set of states $\{|k\rangle, |j\rangle, |+\rangle \equiv (|k\rangle + |j\rangle)/\sqrt{2}, |+_y\rangle \equiv (|k\rangle + i|j\rangle)/\sqrt{2}\}$, namely [54],

$$|k\rangle\langle j| \equiv |+\rangle\langle +| + i|+_y\rangle\langle +_y| - \frac{(i+1)}{2}(|k\rangle\langle k| + |j\rangle\langle j|),$$

and then exploit the linearity property of any closed quantum dynamics.

We close this section with some remarks.

Remark 4. We have shown that the interaction Hamiltonian (and consequently the topology) of an autonomous quantum dynamical network is identifiable also by properly processing the information coming from partial measurements of ρ_t (in particular, its diagonal elements), provided that d^2 linearly independent initial states are prepared. Such initial states have quantum coherence contributions (corresponding to off-diagonal terms in ρ_0) between the elements of the basis chosen for their decomposition. Thus, for an accurate reconstruction of the network topology, decreasing the number of intermediate measurements necessarily entails an increase in the complexity of the initial quantum state preparation.

Remark 5. Proposition 2 applies also to quantum networks composed of N interacting ℓ-level quantum subsystems. For such systems, indeed, the Liouville–von Neumann equation in linear form can be written as $\dot{\boldsymbol{\lambda}}_t = (\mathcal{L}_0 + \mathcal{L}_{\text{int}})\boldsymbol{\lambda}_t$, where $\mathcal{L}_0 \equiv -\frac{i}{\hbar}\widetilde{H}_0$ and $\mathcal{L}_{\text{int}} \equiv -\frac{i}{\hbar}\widetilde{H}_{\text{int}}$. Under the assumptions of Proposition 2 [observability of the pair $(C, \mathcal{L})$ and linearly independent initial states], it is guaranteed that the operator $\mathcal{L}_0 + \mathcal{L}_{\text{int}}$ can be uniquely identified. Therefore, with $\mathcal{L}_0$ being fixed and known *a priori*, Proposition 2 ensures that also $\mathcal{L}_{\text{int}}$ is **uniquely** identifiable.

Remark 6. Since the quantum network Hamiltonian is the quantity to be determined, *a priori* it is unknown if the pair $(C, \mathcal{L})$ is observable. This means that, in general, it is not guaranteed that a possible solution $\hat{M}$ of the topology identification problem is reliable and accurate. Accordingly, for practical purposes it is worth checking *a posteriori* the observability of the pair $(C, \hat{\mathcal{L}})$, with $\hat{\mathcal{L}} \equiv -\frac{i}{\hbar}(\mathbb{I}_d \otimes \hat{M} - \hat{M}^T \otimes \mathbb{I}_d)$, which is computed by taking the solution $\hat{M}$ of the identification problem.

VII. CONCLUSIONS

In this paper we have addressed the issue of determining under which analytical conditions it is possible to identify the topology of an autonomous quantum network. Specifically, we provide a procedure for the reconstruction of quantum network topologies by using the full information of the network density operator ρ_t, even taken at discrete times. As already discussed in the introductory part of the paper, solutions to this problem could find application in quantum computing and quantum communication, where multiple quantum devices need to be connected in network configurations. In such contexts, information on the network topology is not always available and, as for any other network whose nodes are dynamical systems, even for a quantum network it can happen that one of the nodes looses its functionality or some links suddenly break down. Hence, in all these cases, reliable and easy-to-use tools for topology identification are a prerequisite.

To achieve our goal in solving the topology reconstruction problem, we have assumed to be able to measure the density operator ρ_t of the network over a given time interval. In particular, we have considered measuring both all the elements of ρ_t, for example, by means of quantum state tomography, and only a part of them (just the diagonal elements of ρ_t). Though the former case (identification with *full* information) requires more entries of ρ_t to be measured than the latter (identification with *partial* information), we provide a sufficient condition for the solvability of the problem by inverting an algebraic commutation relation. This means that if the identification problem is solvable, the quantum network topology can be reconstructed, in principle, with zero error. The analytical conditions that allow to the identification problem to be solved with full information have been then converted in a reconstruction algorithm (Algorithm 1). Algorithm 1 does not require high computing power, and it can be implemented on standard computer facilities. However, one may encounter the issue of computing with few resources (thus, approximately) the operator P, obtained by integrating ρ_t within the time interval $[0, \tau]$. The accuracy in calculating this integral depends on the number of time-discrete data points of ρ_t in $[0, \tau]$. In this regard, since at the experimental level the effort in performing lots of measurements is prohibitive, we have numerically verified whether the solvability of the topology identification problem with full information is still guaranteed by decreasing the accuracy in computing P, namely, by using a smaller number of samples. The identification problems remain solvable, though the reconstruction error ϵ tends to become high, especially if the number of nodes is large or with a too small value of the duration τ of the quantum network evolution.

Finally, we have addressed the problem to identify a quantum network topology by using measurements of only the diagonal elements of ρ_t. Specifically, here we have shown that the topology of an autonomous quantum network might be reconstructed if the network is observable and is initialized on d^2 linearly independent initial states in different runs.

The procedures addressed here for the topology identification of autonomous quantum dynamical networks have to be considered *causal*, in the sense that at any time t (when the functionality of the procedure is evaluated) we process information available up to $t \in [0, \tau]$, thus without employing any information on the state (or any observable) depending on a time instant $t' > t$. Moreover, we also stress that, for a possible experimental implementation of the procedure, our identification routine needs to be restarted from the beginning every time that information on the quantum network state is measured and then collected. Such a strategy may be quite resource consuming, but it can avoid resorting to ancillary quantum systems.

With other contributions (one can, for example, refer to the review paper [55]), our paper is one of the attempts to apply analytical results from control theory to quantum-mechanical systems. One of our purposes, indeed, is to stimulate contributions that aim at providing exact results in the quantum engineering interdisciplinary field.

Although our analysis has dealt with several facets of the topology identification problem for autonomous quantum networks, it certainly cannot be considered exhaustive. Let us thus mention some others: (i) A more extensive numerical analysis for the testing of our topology identification procedure to connected quantum networks whose links follow nonstandard topologies. For this purpose, one could test random quantum networks with links sampled from known generalizations of the Erdős-Rényi probability distribution. (ii) Extension of the obtained analytical and numerical results to the case of nonautonomous (or driven) quantum networks. (iii) Solution of the addressed topology identification problem for open quantum networks in interaction with an external environment or other quantum systems.

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APPENDIX A: INTERPRETING A MANY-BODY QUANTUM SYSTEM AS A QUANTUM NETWORK

Let us consider an ensemble of N interacting ℓ-level quantum systems, each of them characterized by its own time evolution. Such a many-body quantum system is closed, namely, it does not interact with the surroundings. As a consequence, the dynamical evolution of the global system is unitary and governed by the total Hamiltonian H. As provided by Eq. (5) in the main text, H is given by the sum of

the Hamiltonian operators of each subsystem with interaction terms describing the coupling between the subsystems. Formally, $H = \sum_k \omega_k H_k + H_{\rm int}$, with k the index on the network subsystems. By assuming (as in the main text) the presence of only two-body interactions and compositions of them at any $t \in [0, \tau]$, the interaction Hamiltonian $H_{\rm int}$ can be further decomposed as the sum of $D \equiv N(N-1)$ coupling terms $A_k A_j$ with $k \neq j$. Each of them corresponds to a link between two distinct quantum subsystems of the quantum network. Thus $H_{\rm int} = \sum_{k \neq j} \alpha_{k,j} A_k A_j$.

Now, as a further element, let us observe that also each operator A_k, with $k = 1, \ldots, N$, can be decomposed as the sum of characteristic operators and specifically as the sum of $\ell^2 - 1$ eigenoperators, constituting a complete orthonormal basis of the node Hamiltonian operators H_k, i.e.,

$$A_k = \sum_{n=1}^{\ell^2-1} \beta_n A_k^{(n)} \quad \text{subject to} \quad \sum_{n=1}^{\ell^2-1} A_k^{(n)} = \mathbb{I}_d.$$

Accordingly, the interaction Hamiltonian $H_{\rm int}$ equals

$$H_{\rm int} = \sum_{k,j=1;k\neq j}^{N} \sum_{n_1,n_2=1}^{\ell^2-1} \gamma_{k,j,n_1,n_2} A_k^{(n_1)} A_j^{(n_2)},$$

where $\gamma_{k,j,n_1,n_2} \equiv \alpha_{k,j}\beta_{n_1}\beta_{n_2}$. For convenience, it is worth introducing the index m that labels the links of the networks. Note that in this analysis both the links $k \to j$ and $j \to k$ are distinct elements, generally with a different weight. For example, this means that $m = 1$, $m = N-1$, and $m = N(N-1)$ correspond, respectively, to the 2-tuples $(k = 1, j = 2)$, $(k = 1, j = N)$, and $(k = N, j = N-1)$. As a result, $H_{\rm int}$ can be written as the sum of $D_2 \equiv (\ell^2-1)^2 N(N-1)$ elements as in the following relation:

$$H_{\rm int} = \sum_{m=1}^{N(N-1)} \sum_{n_1,n_2=1}^{\ell^2-1} \gamma_{m,n_1,n_2} B_{m,n_1,n_2},$$

with $B_{m,n_1,n_2} \equiv A_k^{(n_1)} A_j^{(n_2)}$, and $n_1, n_2 = 1, \ldots, \ell^2 - 1$, $m = 1, \ldots, N(N-1)$.

In conclusion, by substituting the expression of $H_{\rm int}$ in H, the Liouville–von Neumann equation of a quantum many-body system interpreted as a quantum network is equal to

$$\dot{\rho}_t = -\frac{i}{\hbar}[(H_0 + \boldsymbol{\gamma}^T E \boldsymbol{\gamma}), \rho_t] = R_0 - \frac{i}{\hbar}[\boldsymbol{\gamma}^T E \boldsymbol{\gamma}, \rho_t],$$

where R_0, as in the main text, is completely determined by the knowledge of the local dynamics of each ℓ-level quantum system, while $\boldsymbol{\gamma}$ and E are provided by the relations

$$\boldsymbol{\gamma} = \left(\sqrt{\gamma_{1,1,1}}\,\mathbb{I}_d, \ldots, \sqrt{\gamma_{m,n_1,n_2}}\,\mathbb{I}_d, \ldots\right)^T \in \mathbb{C}^{D_2 d \times d}$$
$$E = \mathrm{diag}\left(\{B_{m,n_1,n_2}\}\right) \in \mathbb{C}^{D_2(d\times d)}.$$

The latter formulas for $\boldsymbol{\gamma}$ and E correspond to the ones for $\boldsymbol{\alpha}$ and C in Sec. II of the main text.

APPENDIX B: PROOF OF THEOREM 1

Let $M \in \mathcal{A}_\rho$. By integration of the Liouville–von Neumann equation $\dot{\rho}_t = -\frac{i}{\hbar}[M, \rho_t]$ between $t = 0$ and $t = \tau$, Eq. (12) of the main text is obtained. By hypothesis, we have assumed the existence of a unique $\hat{M} \in \mathcal{A}$ satisfying Eq. (12). As a consequence, $|\mathcal{A}_\rho| = 1$, meaning that the set $\mathcal{A}_\rho$ contains only a single element. Thus, since by construction $H \in \mathcal{A}_\rho$, we can conclude that $\mathcal{A}_\rho = \{H\}$.

APPENDIX C: PROOF OF PROPOSITION 1

To demonstrate the "if" statement, let us assume that $\hat{M}_1, \hat{M}_2 \in \mathcal{A}$ are solutions to Eq. (12). Clearly, we have $(\hat{M}_1 - \hat{M}_2) \in \mathcal{A}$. In addition, we obtain

$$(\hat{M}_1 - \hat{M}_2)P - P(\hat{M}_1 - \hat{M}_2) = 0,$$

that is, $\hat{M}_1 - \hat{M}_2$ commutes with P. Thus by hypothesis we obtain $\hat{M}_1 = \hat{M}_2$, i.e., there is a unique solution to (12) in the set $\mathcal{A}$. Conversely, to prove the "only if" statement, let $Z \in \mathcal{A}$ commute with P. This implies that $\hat{M} \equiv H + Z \in \mathcal{A}$ is a solution to (12). Since this solution is unique by hypothesis, we obtain $Z = 0$, which proves the "only if" statement and thus the theorem.

APPENDIX D: PROOF OF PROPOSITION 2

Suppose that both the pairs $(C, \mathcal{L})$ and $(C, \overline{\mathcal{L}})$ generate the outputs $\boldsymbol{y}_{\lambda_0^{(\ell)}}(t)$ for $t \in [0, \tau_\ell]$, $\tau_\ell > 0$, and $\ell = 1, \ldots, d^2$. Moreover, let us recall that by construction $\dot{\boldsymbol{\lambda}}_t = \mathcal{L}\boldsymbol{\lambda}_t$ and $\boldsymbol{y}_t = C\boldsymbol{\lambda}_t$ for any value of t. Thus one can find that

$$\dot{\boldsymbol{y}}_{\lambda_0^{(\ell)}}(0) = C\mathcal{L}\boldsymbol{\lambda}_0^{(\ell)} = C\overline{\mathcal{L}}\boldsymbol{\lambda}_0^{(\ell)}.$$

In similar fashion, by computing higher-order derivatives of $\boldsymbol{y}_t$ until the d^2-th one, we also get

$$C\mathcal{L}^k\boldsymbol{\lambda}_0^{(\ell)} = C\overline{\mathcal{L}}^k\boldsymbol{\lambda}_0^{(\ell)}$$

for all $k = 1, 2, \ldots, d^2$. Since the initial states $\boldsymbol{\lambda}_0^{(\ell)}$, with $\ell = 1, 2, \ldots, d^2$, are linearly independent vectors, it holds that $C\mathcal{L}^k = C\overline{\mathcal{L}}^k$ for all $k = 1, 2, \ldots, d^2$. Hence,

$$\begin{bmatrix} C \\ C\mathcal{L} \\ \vdots \\ C\mathcal{L}^{d^2-1} \end{bmatrix} \mathcal{L} = \begin{bmatrix} C \\ C\overline{\mathcal{L}} \\ \vdots \\ C\overline{\mathcal{L}}^{d^2-1} \end{bmatrix} \overline{\mathcal{L}} = \begin{bmatrix} C \\ C\mathcal{L} \\ \vdots \\ C\mathcal{L}^{d^2-1} \end{bmatrix} \overline{\mathcal{L}}.$$

Equivalently,

$$\begin{bmatrix} C \\ C\mathcal{L} \\ \vdots \\ C\mathcal{L}^{d^2-1} \end{bmatrix} (\mathcal{L} - \overline{\mathcal{L}}) = 0.$$

Finally, by resorting to the assumption that the pair $(C, \mathcal{L})$ is observable, we can conclude that $\mathcal{L} = \overline{\mathcal{L}}$, thus proving the Proposition.

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