

Harnessing Intrinsic Noise for Quantum Simulation of Open Quantum Systems

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Simulating open quantum systems on quantum computers presents a fundamental challenge: open quantum dynamics are intrinsically nonunitary, whereas quantum computers operate through unitary evolution. Conventional approaches overcome this mismatch by encoding nonunitary processes into unitary circuits, but such methods incur substantial overhead in both qubits and gates. Here, we propose an alternative perspective. Quantum processors are themselves open systems, inherently subject to noise. Instead of correcting all errors and then encoding nonunitary dynamics with unitary logical qubits and gates, we show how noise can be harnessed as a computational resource. We develop a noise-assisted quantum algorithm that selectively preserves physical noise to emulate nonunitary channels, enabling efficient simulation of open quantum dynamics with minimal qubit requirements. Our approach applies both to noisy intermediate-scale quantum (NISQ) devices and future fault-tolerant architectures. By leveraging intrinsic noise, this method circumvents the need to encode nonunitary dynamics into unitary gates and relaxes fidelity requirements on physical qubits, thereby reducing the overhead of quantum error correction. This framework reframes noise from a limitation into a resource, opening new directions for practical quantum simulation of open systems

I. INTRODUCTION

In realistic conditions, a quantum system inevitably interacts with its bath (or environment), forming an *open quantum system*. Consequently, the study of open quantum dynamics is essential to explore the properties and behaviors of molecules, materials, and quantum devices under experimentally relevant conditions. Unlike static properties, dynamical simulations capture transient behavior [1–3], reveal kinetic effects [4, 5], and elucidate non-equilibrium processes such as transport [6–8], and quantum decoherence [9–14]. They play a significant role in studying complex properties of driven systems [15–19], analyzing quantum information flow [20–24], and developing quantum technologies including sensors [25–31], transducers [32–36], and simulators [37–44]. However, accurate simulation of open quantum dynamics is notoriously challenging [45–48], as the Hilbert space required to represent a quantum state grows exponentially with the system size, rapidly surpassing the classical limits.

State-of-the-art algorithms on classical computers like Density Matrix Renormalization Group (DMRG) [49], Multi-Configurational Time-Dependent Hartree (MCTDH) [50, 51], tackle this challenge by truncating the Hilbert space via low-rank approximation [52]. Although these techniques are effective in certain low-dimensional or weakly entangled systems, they struggle with high-dimensional, strongly correlated, or long-range interacting systems [53]. In addition, Hierarchical equations of motion (HEOM) [54, 55] offer a technique to perform quantum simulations without the

standard simplifying assumptions like the Born, Markovian, and Rotating Wave approximations. However, this suffers from a large computational cost as the system scales up. Moreover, at low temperatures, convergence of the Matsubara expansion requires many terms that dramatically increases the hierarchy depth and makes simulations extremely expensive [56, 57]. As a result of these drawbacks, the simulation of many realistic open quantum dynamics problems often falls beyond reach.

Richard Feynman proposed in 1982 that quantum computers offer the most natural platform for modeling quantum systems, including quantum dynamics [58]. Because the accessible state space grows exponentially with the number of qubits, quantum computers possess enormous expressive power in Hilbert space. The promise of efficiently simulating quantum systems stimulated the development of quantum algorithms for energy estimation and quantum dynamics [59–66]. However, performing such simulations is not a trivial task, as quantum computers are extremely fragile processors and are affected by thermal, chemical, electromagnetic, and other fluctuations that arise from the bath they are placed in. These noise sources can drive the output state from the intended target, necessitating quantum error-correction (QEC) codes that assemble high-fidelity logical qubits from large numbers of physical qubits [67, 68].

On the other hand, quantum algorithms for open quantum system dynamics face a fundamental mismatch: (fault-tolerant) quantum computers are inherently unitary, while open quantum system dynamics are nonunitary. One such technique to address this is Hilbert-space dilation [69] by adding ancilla qubits that emulate bath degrees of freedom and simulate the unitary dynamics of the enlarged system. Other strategies explored in the literature include unitary decompositions [48], analog quan-

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tum simulation [70], and pseudo-identity unitary transformations [71], among others. Yet these approaches often demand additional qubits and deep circuits, compounding hardware overhead and error susceptibility.

In this work, we ask a different question: rather than suppressing all noises and nonunitary effects to restore perfectly unitary logical evolution, can we leverage the inherent nonunitary dynamics of noisy qubits, whether physical qubits or lower-fidelity logical qubits, to emulate the nonunitary evolution of open quantum systems? We address this question by developing a new approach that avoids ancillary dilation by constructively encoding a system's decoherence channels and averaging hardware noise into a computational resource. By partially encoding a system's decoherence channels, we harness the intrinsic noise present in real quantum hardware to emulate the nonunitary aspects of open-system evolution. This strategy offers two key advantages: (i) it relaxes the requirement for ultra-high-fidelity logical qubits, lowering the physical-qubit and gate overhead of QEC, i.e., only the error components that exceed or mismatch the desired dissipation need to be corrected; and (ii) it bypasses the need to embed nonunitary evolution into unitary dynamics. Moreover, we also show that the intrinsic noise triggers the formation of clusters of partially encoded system channels. These clusters act as decoherence-free subspaces (DFSs) [72–79] that can also be used as resources when performing quantum simulations.

The paper is organized as follows: Sec. II introduces the theory surrounding open quantum system dynamics as seen in physical systems and outlines our algorithms for encoding the system's decoherence channels on a quantum circuit utilizing the intrinsic noise of a quantum computer. To formalize these arguments, we take inspiration from the Choi-Jamiołkowski isomorphism and introduce a practical bound on the residues of our algorithm in Sec. II E. Furthermore, we discuss the performance of our algorithms in Sec. III. We do this by first analyzing the convergence of our algorithm to match the decoherence channels in Subsec. ??, and then benchmark this by simulating the coherent-dissipative energy transport in a multi-exciton model in Subsec. III B. Finally, in Sec. IV, we summarize our results and discuss their implications.

II. THEORY

The Hamiltonian of an open quantum system S interacting with a bath B can be expressed as

$$H_T = H_S + H_B + H_{SB}, \quad (1)$$

where H_S , H_B , and H_{SB} denote the Hamiltonians of the system, the bath, and the system–bath interaction, respectively. The dynamics of the open quantum system can be derived by tracing out the bath degrees of freedom (DOFs) from the unitary dynamics of the entire system

H_T . One widely used formalism for the Markovian dynamics is the quantum Lindblad master equation [9–13] (with $\hbar = 1$),

$$\frac{\partial \rho}{\partial t} = i[\rho, H_S] + \sum_i \left(\Gamma_i \rho \Gamma_i^\dagger - \frac{1}{2} \Gamma_i^\dagger \Gamma_i \rho - \frac{1}{2} \rho \Gamma_i^\dagger \Gamma_i \right). \quad (2)$$

The first term on the right-hand side contributes to the unitary dynamics of the system, while the second term contributes to the nonunitary dynamics arising from the coupling of the system with the bath degrees of freedom.

Beyond Markovianity, the dynamics of open quantum systems are generally formulated in the so-called Kraus representation [9]

$$\mathcal{E}(\rho) = \sum_i K_i \rho K_i^\dagger, \quad (3)$$

where K_i are the Kraus operators satisfying the completeness relation $\sum_i K_i^\dagger K_i = \mathbb{I}$ and form a completely positive trace-preserving (CPTP) map [9]. The Kraus formalism can be readily derived from the unitary dynamics of the entire system by tracing out the bath degrees of freedom. Note that when $K_0 = \mathbb{I} - (iH_S + \frac{1}{2} \sum_i L_i^\dagger L_i) \Delta t$ and $K_i = \sqrt{\Delta t} L_i$, Eq. (3) reduces to the Lindblad formalism (Eq. (2) with $L_i = \Gamma_i$) as $\Delta t \rightarrow 0$.

One usually employs Pauli twirling to convert the noise described by the Kraus operators into Pauli strings, which is given by

$$\mathcal{E}(\rho) = \sum_i w_i P_i \rho P_i, \quad (4)$$

where $P_i \in \{I, X, Y, Z\}^{\otimes n}$ is the n -qubit Pauli group under matrix multiplication, with $\sum_i w_i = 1$. We observe that Eq. (4) converts a pure state into a mixed state and agrees well with the dynamics of open quantum systems. Such behavior is also replicated in current noisy intermediate-scale quantum (NISQ) devices, where noise converts any pure input state into highly mixed output states. Since we are interested in simulating the dynamics of an open quantum system on a quantum computer, we describe the decoherence channels of an open quantum system in a similar vein as:

$$\mathcal{E}_{\text{sys}}(\rho) = \sum_i w_i P_i \rho P_i \quad (5)$$

and the intrinsic noise channels of qubits of arbitrary hardware as,

$$\mathcal{E}_I(\rho) = \sum_k w_k P_k \rho P_k^\dagger. \quad (6)$$

This holds true since the intrinsic noise channels are decoherence channels of a quantum processor that is coupled to a bath. To simulate a system that obeys this equation on a quantum computer, we need to encode the system's degrees of freedom onto qubits and encode

the dynamics as gates on the quantum computer. Oftentimes, the sets $\{P_i\} \neq \{P_k\}$ and $\{w_i\} \neq \{w_k\}$. This means that the intrinsic noise channels that affect a quantum computer are different from the decoherence channels that affect an open quantum system. In this work, we delineate a scheme that uses these intrinsic noise channels of a QC to simulate open quantum dynamics by employing partial encoding of the system's decoherence channels. In particular, we assume that a single-/two-qubit noise channel is triggered when a single-/two-qubit gate is applied in a circuit. We also note that, in this process, some channels get overly encoded or cannot be partially encoded in the algorithm. In such cases, we employ a partial error correction technique that forms a future aspect of this work. To demonstrate the partial encoding technique, we begin by outlining the scheme for single-qubit channels and later expand it to two- and multi-qubit channels.

A. Partial Encoding of Single-Qubit channels

In the presence of single-qubit noise, the Pauli strings from Eqs. (4) and (6) simplify to Pauli operators, $P \in \{X, Y, Z, I\}$. When a system channel, P_i , is implemented as a gate on a quantum circuit, the intrinsic noise effectively encodes a weighted sum of channels within this set. This gives rise to three processes depending on the intrinsic noise and the channels present in the system:

1. *Complete encoding of a system channel:* This occurs when the intrinsic noise converts the encoded gate into an effective channel that is not present in the system. In such a scenario, we completely encode the channels present in the system and partially correct the resulting channels that arise from the effects of intrinsic noise.
2. *Partial encoding of a system channel:* This occurs when the intrinsic noise converts the encoded gate into effective channels that are partly or completely present in the set of system channels. In such a scenario, we employ an iterative partial encoding scheme to systematically encode all the system channels onto the quantum computer.
3. *Partial error correction:* This is a carefully selected process that eliminates any unwanted channels that are encoded on the quantum circuit.

The effective channel that is implemented on the quantum circuit can also be expressed as a sum of Pauli operators as in Eq. (4). We calculate the differences between the effective channel and the target system channel and call it the residue. Lastly, we feed this residue back into the target channels and repeat this process until all residues converge to zero. At this point, all system channels will have been encoded on the quantum processor using the intrinsic noise. For the sake of brevity, and for

the reason that two-qubit gate noise channels dominate over single-qubit gate noise channels in most quantum processors, we reserve the elaboration of the above procedure in Sec. II B.

B. Partial Encoding of Two-Qubit Channels

The predominant sources of noise in quantum computers arise from the implementation of two-qubit gates. In literature, one often characterizes the depth of a quantum circuit and, consequently, benchmarks quantum algorithms by counting the number of CNOT gates that are implemented. These implementations are usually imperfect and noisy, and we can write the gate implementation channel as in Eq. (6) with $n = 2$ qubits. Under two-qubit noise, the Pauli group contains 16 channels. Analogous to the arguments presented in Sec II A, the encoding of a two-qubit system channel as a unitary gate triggers the two-qubit intrinsic noise channels. This results in an effective mapping to a new channel that may/may not be present in the system. Concretely, this mapping is given by

$$\{w_i, P_i\}_S \xrightarrow{\{w_j, P_j\}_I} \{\tilde{w}, \tilde{P}\}_{\text{eff}}, \quad (7)$$

where the sets $\{w_i, P_i\}_S$ and $\{w_j, P_j\}_I$ are the set of weighted Paulis from Eqs. (5) and (6). However, since these mappings are the results of products of Pauli matrices, they are cyclic under matrix multiplication given by $\sigma^i \cdot \sigma^j = 2i\epsilon_{ijk}\sigma^k$. This means that any set of intrinsic Pauli noise, $\{P_j\}_I \in \{X, Y, Z, I\}_I^{\otimes 2}$, generates a closed subspace within the 2-qubit Pauli group of the system. Physically, this implies that if we encode any channel from the set $\{P_i\}_S \in \{X, Y, Z, I\}_S^{\otimes 2}$, the intrinsic noise $\{P_j\}_I$ generates a decoherence-free subspace (DFS) within the configuration space of the system since all the mappings are closed within this group.

Fig. 1a) shows an example of the two-qubit bit-flip noise X_1X_2 generating a closed map between the X_1Z_2 and I_1Y_2 system channels. Encoding either of the channels under the bit-flip noise will confine the iterative process within this subspace and will not produce new channels. This partial encoding scheme reduces the amount of error correction required in later stages of the algorithm. Fig. 1b) gives an example of the intrinsic noise $\{X_1X_2, Y_1, Y_2, Z_1, Z_2\}_I$ generating a closed map between the elements of the set $\{Y_1I_2, Z_1X_2, X_1Z_2, I_1Y_2\}_S$ of system channels. In each of these examples, one can identify a nodal channel that branches out to multiple channels. This node is the channel encoded as a gate in the quantum circuit and maps to itself under the I_1I_2 intrinsic noise with probability equal to the corresponding magnitude. An example of such a node is Y_1I_2 in Fig. 1b) where we see three channels branching out of it as indicated by the blue arrows. Note that these branches are reversible up to a global phase. This phase can be ignored since they cancel out in Eq. (4). The yellow

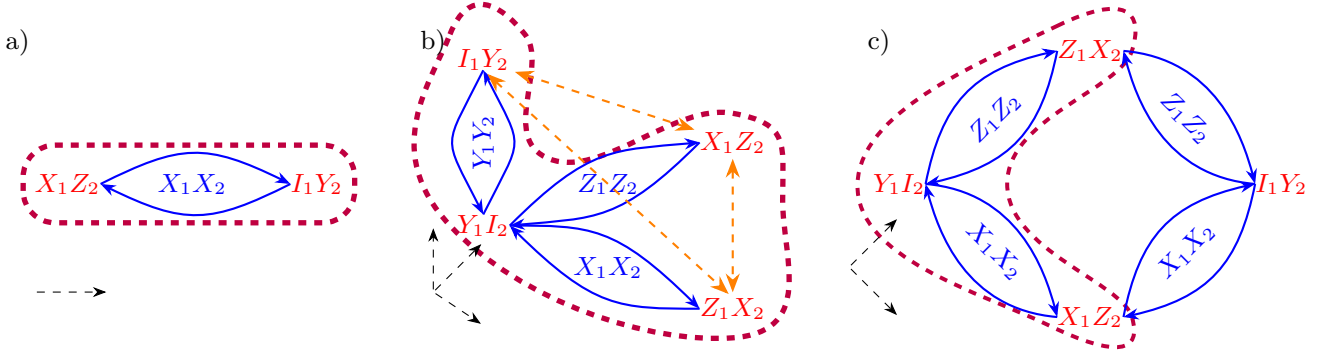


FIG. 1. a) 1D braiding structure with $n = d + 1$. b) 3D braiding with the Y_1I_2 nodal channel. This braiding generates a decoherence-free subspace for the exemplified $\{Y_1I_2, I_1Y_2, X_1Z_2, Z_1X_2\}$ system channels under the $\{X_1X_2, Y_1Y_2, Z_1Z_2\}$ channels. Blue arrows indicate mapped channels; yellow arrows indicate alternate choices that preserve the DFS while maintaining the $n = d + 1$ structure. c) The simplest example of the braiding structure $((n, d))$, $n > d$. Here $n = 4$, $d = 2$. This does not generate an all-to-all mapping since the absence of Y_1Y_2 does not close the DFS. The black arrows in each subfigure denote the branches emerging out of a selected node and highlight the braiding dimension.

arrows are branches that correspond to alternate nodal selections and reinforce the generation of a DFS with all-to-all mappings of the system channels.

Having defined a nodal channel and recognized its importance within an iteration in the algorithm, we define a d_b -dimensional braiding shown by the purple dashed lines in each subfigure of Fig. 1. This braiding process can be seen as a thread that originates from one of the nodes and binds all the channels that are immediately connected to it. The dimension d_b is the number of channels that the process covers, excluding the node. Without loss of generality, we identify that the braiding structure and dimension are invariant of the node selection and merely depend on the number of intrinsic noise channels. We also identify that the dimension of braiding need not be the same as the dimension of the DFS generated. As a simplest example, consider the generation of a DFS under the noise $\{X_1X_2, Z_1Z_2\}$, in Fig. 1c). A node in this figure maps to two other channels as shown by the $d_b = 2$ dimensional braiding. However, the noise channels create a cyclic map between 4 system channels, all of which are not present in a single realization of a braiding. We define the dimension, d_c , of this DFS as the number of elements present in it and note that $d_c = 4 \neq d_b = 2$. In particular, as we generalize to multiple noise channels, we find that $d_c \geq d_b + 1$ where the equality holds for noise channel sets that contain symmetric elements and generate all-to-all mappings in the DFS. Examples of such symmetric sets are the limiting sets, $\{X_1X_2\}/\{Y_1Y_2\}/\{Z_1Z_2\}$ and $\{X, Y, Z, I\}^{\otimes 2}$ where the identity channels are implied. Fig. 1b) demonstrates one such instance of an $d_c = d_b + 1$ DFS structure generated by 3 symmetric set of noise channels. Consequently, we can categorize the DFSs generated into two classes: (i) $d_c = d_b + 1$ braiding structured DFSs, and (ii) $d_c > d_b + 1$ braiding structured DFSs.

In the adaptive encoding scheme that follows in Sec. IID, we use the properties of these classes to in-

form the development of our algorithm. Developing such an adaptive encoding algorithm for the latter becomes nontrivial since the entropy, $S = k \cdot \ln\left(\frac{d_c}{d_b+1}\right)$, of the braiding structure is high. Here, $d_c/(d_b + 1)$ gives the number of braiding structures present within a DFS and can be interpreted as microstates that contribute to the entropy of the DFS. This reduces to $S = 1$ for noise channel sets that are symmetric. Figs. 1a)-b) correspond to the $d_c = d_b + 1$ braiding structure while Fig. 1c) is the simplest example of the $d_c > d_b + 1$ braiding structure.

The properties and discussion listed so far can be summarized in the 2-qubit partial encoding algorithm given in Algorithm 1.

Algorithm1 Partial encoding of two- and n-qubit channels

- 1: **Require:** System channel $\mathcal{E}_{\text{sys}}(\rho) = \sum_k p_k P_k \rho P_k^\dagger$, and intrinsic noise channel $\mathcal{E}_I(\rho) = \sum_i w_i P_i \rho P_i^\dagger$, with $P_k, P_i \in \{X, Y, Z, I\}^{\otimes 2}$
 - 2: **Ensure:** $\sum_k p_k = \sum_i w_i = 1$
 - 3: Define $S = \{(p_k, P_k) \mid k \in [0, 15]\}$ from $\mathcal{E}_{\text{sys}}$
 - 4: Define $I = \{(w_i, P_i) \mid i \in [0, 15]\}$ from $\mathcal{E}_I$
 - 5: Choose subset $s = \{(p_l, P_l)\} \subset S$ $\triangleright$ This is the nodal channel. One can trivially take $l = 0$.
 - 6: **for** each iteration i **do**
 - 7: Encode s on the quantum circuit using Pauli gates
 - 8: Compute the effective channel: $\mathcal{E}_{\text{eff}}(\rho) = \sum_i \tilde{w}_i \tilde{P}_i \rho \tilde{P}_i^\dagger$ such that $\tilde{w}_i = p_l w_i$ and $\tilde{P}_i = P_i P_l$.
 - 9: Set $\tilde{s} = \{(\tilde{w}_k, \tilde{P}_k) \mid \tilde{w}_k \neq 0\}$
 - 10: Compute residue: $\Delta^{(i)} = \{(p_k - \tilde{w}_k, P_k)\}$
 - 11: Update $S \leftarrow \Delta^{(i)}$
 - 12: **end for**
 - 13: **return** Circuit that encodes $\mathcal{E}_{\text{eff}}(\rho) \approx \mathcal{E}_{\text{sys}}(\rho)$
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C. Generalization to Multiple Qubits

The Algorithm 1, Fig. 1, and the ideas developed in Sec. II B constitute the foundation of our partial encoding scheme. However, quantum processors consist of multiple qubits and more complex intrinsic noise channels than previously considered. These noise channels can vary in strength across qubits and can also be architecture-dependent. More specifically, the ability of a quantum hardware to implement a multi-qubit gate is dependent on its coupling map. Consequently, this affects the kinds of intrinsic noise channels that arise in a quantum processor. To accommodate these complexities, we observe that the gate implementation abilities in current state-of-the-art hardware are upper-bounded by two-qubit gates. This is because gates acting on more than two qubits are harder to implement and are accompanied by larger noise that can be challenging to correct in order to derive quantum advantage. Moreover, any multi-qubit gate can be decomposed into single- and two-qubit basis gates that adhere to the coupling map and modality of the underlying hardware.

With this motivation, we assume that a quantum processor implements only single- and two-qubit gates or transpiles multi-qubit gates into single- and two-qubit gates. As a result, we consider multi-qubit noise channels with non-identity noise acting on at most two qubits. The intrinsic noise channel from Eq. (6) can then be written as,

$$\mathcal{E}_I^{(2)}(\rho) = \sum_k w_k P_k \rho P_k^\dagger \quad (8)$$

with

$$P_k \in \{P\}^N := \mathbf{P} \left[\{X, Y, Z, I\}^{\otimes 2} \otimes I^{\otimes (N-2)} \right], \quad (9)$$

where N is the number of qubits in the hardware, $\mathbf{P}$ denotes a permutation of the constituent terms of the set, and the superscript (2) denotes that the noise channel is upper bounded by two-qubit gates. We now define the set $\{P\}_{nn}^N$ as,

$$\{P\}_{nn}^N := \mathbf{P}_{nn} \left[\{X, Y, Z, I\}^{\otimes 2} \otimes I^{\otimes (N-2)} \right], \quad (10)$$

where $\mathbf{P}_{nn}$ permutes the terms in the square brackets such that the first set of tensor product of two operators permutes as a whole with the individual components of the second set of $N - 2$ identity operators. With this constraint, we identify that $\{P\}_{nn}^N \subset \{P\}^N$. Physically, this means that every two-qubit gate that triggers the intrinsic noise is implemented as a nearest-neighbor instruction. This form is well-motivated because most quantum processors, with various modalities, are able to implement nearest-neighbor two-qubit gates with more efficiency than long-range two-qubit gates. Prominent examples include superconducting quantum processors developed by IBM [80, 81]. To implement the latter,

one usually uses a series of SWAP gates to bring the concerned long-range qubits closer together. This is not only computationally expensive but also harder to implement. For these reasons, we focus our approach on nearest-neighbor gate implementations.

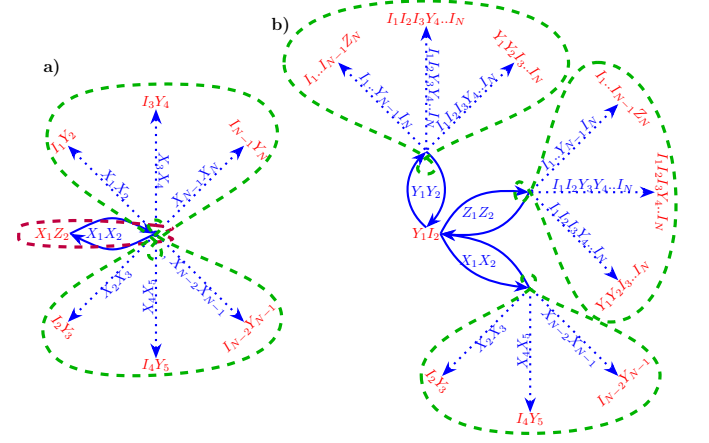


FIG. 2. a) Extension of the 1D braiding to multiple qubits. This figure shows the formation of mutually exclusive sub-clusters under the same intrinsic noise XX for two examples of encoded circuits. b) Extension of the 3D braiding showing cluster formation by the system channels under the presence of three intrinsic noise channels, $\{X_1X_2, Y_1Y_2, Z_1Z_2\}$. This assumes identical nearest-neighbor gate implementations.

Under the formalism described above, we identify the first term in the square brackets of Eq. (10) as the constituents of the intrinsic noise used in Algorithm 1. Since this term consists of only two-qubit Pauli channels, it maps at most two-qubit Paulis at a time from an N -qubit string of the system. The rest of the $N - 2$ identity operators act on the remaining Pauli operators of a system channel and leave it unchanged. This means that for an N -qubit quantum processor (with $N\%2 = 0$), a nodal channel encodes $(m + 1)^{N/2} - 1$ system channels in one iteration, as can be seen in Fig. 2. Here, m is the number of intrinsic noise channels that are triggered when a two-qubit gate is implemented. As shown in Fig. 3a), each ZZ gate maps to YY under noise and ZZ otherwise with probabilities dictated by their corresponding weights in the Pauli noise model. The terms contributing to the resultant density matrix come from the tensor products of each of these YY, ZZ channels. As a result, Figs. 1b) can be extended to Fig. 2b) to show these additional encoded channels as subbranches. We see that, under the same intrinsic noise channels (like XX in Fig. 2), the system channels form clusters indicated by the green clouds. These clusters are analogous to the DFS presented earlier and are extended versions for multiple-qubit channels. Naturally, for $m = 1, N = 2$, this reduces to Fig. 1b).

We emphasize that the simplifying constraint imposed in Eq. (10) is not a necessary condition for the implementation of our technique. This is because we can

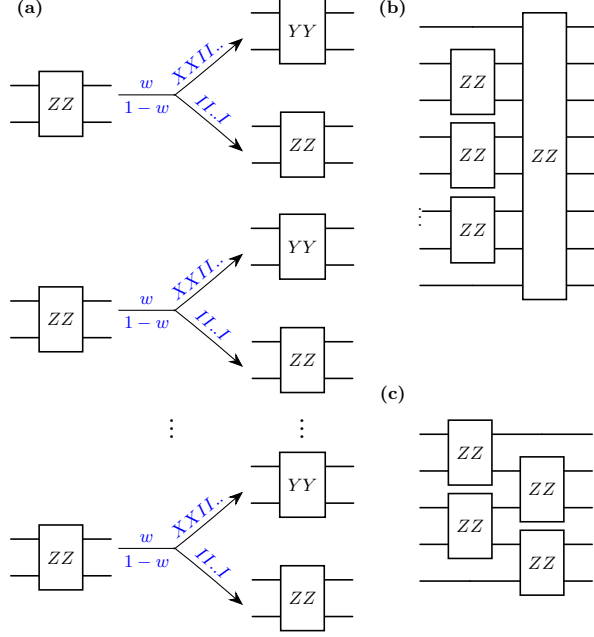


FIG. 3. Examples of two-qubit partially encoded gates: (a) (Nearest-neighbor gates) An example of how the encoded nodal channel $ZZ..Z$ is transformed under the two-qubit intrinsic noise XX . (b–c) Two examples of circuits where the nearest-neighbor gate implementation is relaxed. This gives rise to encoded Pauli strings that are different from those obtained in (a) under the same intrinsic noise XX .

trivially extend it to the more general form in Eq. (8) by allowing the noise to act non-locally and producing more system channels in each of the clusters in Fig. 2b). With these properties in mind, the Algorithm 1 can be trivially generalized to n -qubits by identically applying the identity operator on other sites as described earlier. This leads to the formation of subclusters analogous to the formation of DFS in two-qubits.

D. Adaptive Encoding Scheme

As the diligent reader would observe, the iterative Algorithm 1 presented earlier suffers greatly from over-encoding. This occurs when one or more channels are encoded repeatedly in a quest to converge all residues to 0. As a result, one or more of them diverge to highly negative values and indicate overencoding of the respective system channels. However, this scenario can be mitigated by adaptively encoding the channels at each step of the iteration. This demands an appropriate selection of nodes that mitigate these divergences. Such a nodal selection alters the order in which we encode the system channels in the circuit. However, it can be shown numerically that the output state remains invariant under this ordering, and we can freely choose a node without worrying about it affecting the final density matrix. The

adaptive encoding scheme that we employ to mitigate divergences in the $d_c = d_b + 1$ braiding structure is shown in Algorithm 2.

Algorithm2 Adaptive Encoding Scheme ($n = d + 1$)

- 1: **Require:** System channel $\mathcal{E}_{\text{sys}}(\rho) = \sum_k p_k P_k \rho P_k^\dagger$, and intrinsic noise channel $\mathcal{E}_I(\rho) = \sum_i w_i P_i \rho P_i^\dagger$, with $P_k, P_i \in \{X, Y, Z, I\}^{\otimes 2}$
 - 2: **Ensure:** $\sum_k p_k = \sum_i w_i = 1$
 - 3: Define $S = \{(p_k, P_k) \mid k \in [0, 15]\}$ from $\mathcal{E}_{\text{sys}}$
 - 4: Define $I = \{(w_i, P_i) \mid i \in [0, 15]\}$ from $\mathcal{E}_I$
 - 5: Define a tolerance $tol = 0.1$ that dictates the exit condition of the iteration.
 - 6: **while** $p_k > tol \forall k$ **do**
 - 7: **Adaptive Encoding:** For node selection, pair the highest weighted system Pauli channel with the highest weighted intrinsic noise channel. The nodal channel is then the one that generates the identified system channel using the identified intrinsic noise channel.
 - 8: Define the nodal channel subset $s = \{(p_l, P_l)\}$ as defined above.
 - 9: Encode s on the quantum circuit using Pauli gates
 - 10: Compute the effective channel resulting from the probabilistic composition of the Pauli gates with the intrinsic noise channels.
 - 11: Compute the effective channel: $\mathcal{E}_{\text{eff}}(\rho) = \sum_i \tilde{w}_i \tilde{P}_i \rho \tilde{P}_i^\dagger$ such that $\tilde{w}_i = p_l w_i$ and $\tilde{P}_i |0\rangle = P_i P_l |0\rangle$.
 - 12: Set $\tilde{s} = \{(\tilde{w}_k, \tilde{P}_k) \mid \tilde{w}_k \neq 0\}$
 - 13: Compute residue: $\Delta^{(i)} = \{(p_k - \tilde{w}_k, P_k)\}$
 - 14: Update $S \leftarrow \Delta^{(i)}$
 - 15: **end while**
 - 16: **return** Circuit that encodes $\mathcal{E}_{\text{eff}}(\rho) \approx \mathcal{E}_{\text{sys}}(\rho)$
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E. Bounds on residue distance

Here, we formalize the discussion and algorithms introduced above and derive a practical bound on the residues between the system decoherence channels and those implemented on a quantum processor. Our approach employs the state-channel duality based on the Choi–Jamiołkowski isomorphism [82–84].

Consider a composite Hilbert space $\mathcal{H}_1 \otimes \mathcal{H}_2$ with $d = \dim(\mathcal{H}_1) = \dim(\mathcal{H}_2)$ and a maximally entangled state

$$|\Omega\rangle = \frac{1}{\sqrt{d}} \sum_{i=1}^d |i\rangle \otimes |i\rangle, \quad (11)$$

where $\{|i\rangle\}_{i=1}^d$ forms a complete basis in $\mathcal{H}_1$ or $\mathcal{H}_2$. For a CPTP map $\mathcal{E} : \mathcal{H}_1 \rightarrow \mathcal{H}_1$, the corresponding Choi state is defined as

$$J(\mathcal{E}) = (\mathcal{E} \otimes \mathcal{I})(|\Omega\rangle\langle\Omega|), \quad (12)$$

where $\mathcal{I}$ is the identity operation on $\mathcal{H}_2$. The action of $\mathcal{E}$ on a state ρ is then given by (see Appendix A for details)

$$\frac{1}{d} \mathcal{E}(\rho) = \text{Tr}_2[(\mathbb{I} \otimes \rho^\top) J(\mathcal{E})], \quad (13)$$

where $\mathbb{I}$ is the identity operator and $\top$ denotes matrix transpose.

The system channel and the effective channel implemented on a quantum processor define two CPTP maps acting on $\mathcal{H}_1$. Our goal is to match these two channels, taking the system channel as the target. We denote these maps by $\mathcal{E}_{\text{sys}}$ and $\mathcal{E}_{\text{eff}}$, respectively. We use the operator distance defined by the Schatten p -norm [85, 86], referred to as the *Schatten p -distance* (with $p = 2$ reducing to the Hilbert–Schmidt distance),

$$\|A - B\|_p := \left(\text{Tr} \left[\left((A - B)^\dagger (A - B) \right)^{p/2} \right] \right)^{1/p}. \quad (14)$$

We then obtain bounds on the Schatten p -distance between the system channel and the effective channel on the quantum processor (see Appendix B for the proof),

Theorem 1. Let $J(\mathcal{E}_{\text{sys}})$ and $J(\mathcal{E}_{\text{eff}})$ be the Choi states for the CPTP maps $\mathcal{E}_{\text{sys}}$ and $\mathcal{E}_{\text{eff}}$, respectively. Then for any quantum states ρ acting on d -dimensional Hilbert space, the Schatten p -distance between $\mathcal{E}_{\text{sys}}(\rho)$ and $\mathcal{E}_{\text{eff}}(\rho)$ can be bounded as

$$0 \leq \|\mathcal{E}_{\text{sys}}(\rho) - \mathcal{E}_{\text{eff}}(\rho)\|_p \leq d^2 \|J(\mathcal{E}_{\text{sys}}) - J(\mathcal{E}_{\text{eff}})\|_p \quad (\forall \rho). \quad (15)$$

This theorem provides an alternative demonstration of the state–channel duality through the Choi–Jamiołkowski isomorphism, as it establishes the one-to-one correspondence between $J(\mathcal{E})$ and $\mathcal{E}$ defined by the isomorphism. However, this theorem offers a more *practical* viewpoint, with its primary advantage stemming from the use of the Schatten p -norm, which provides a versatile framework for analyzing properties such as numerical stability and spectral sensitivity. For example, when $p = 2$, the SWAP test can be employed to evaluate the state overlap, thereby yielding the Hilbert–Schmidt distance between two quantum states [87]. In particular, from Eq. (15), if $\|J(\mathcal{E}_{\text{sys}}) - J(\mathcal{E}_{\text{eff}})\|_p \in \mathcal{O}(\varepsilon)$ for arbitrarily small $\varepsilon > 0$, then the channels $\mathcal{E}_{\text{sys}}$ and $\mathcal{E}_{\text{eff}}$ differ by at most $\mathcal{O}(\varepsilon)$, i.e., they are asymptotically close. Consequently, the upper bound $\|J(\mathcal{E}_{\text{sys}}) - J(\mathcal{E}_{\text{eff}})\|_p$ can serve as a cost function, providing a practical and effective metric to achieve perfect partial encoding by iteratively evaluating the efficiently computable Schatten p -distance between the two Choi states.

III. RESULTS AND DISCUSSION

With the background ideas and algorithms outlined above, we analyze the convergence of our algorithm and benchmark it with well-understood classically simulated systems. In Sec. ??, we analyze the convergence of our proposed algorithms, and in Sec. IIIB, we benchmark these algorithms with coherent-dissipative energy transport in molecular aggregates to demonstrate their applications in real open quantum systems.

A. Convergence of the partial encoding algorithm

We begin by demonstrating the convergence of the encoding of a system channel on a quantum computer using its intrinsic noise. Consider the system channels described as follows:

$$\mathcal{E}_{\text{sys}}(\rho) = w_{XZ} XZ\rho XZ + w_{IY} IY\rho IY \quad (16)$$

and the intrinsic noise channel of a quantum computer as,

$$\mathcal{E}_I(\rho) = w_{XX} XX\rho XX + (1 - w_{XX})\rho. \quad (17)$$

Equation (17) says that whenever a system channel, XZ or IY from Eq. (16) (or any other channel), is encoded on a quantum circuit as a two-qubit gate, then the resultant density matrix is affected by the intrinsic noise channel XX with probability w_{XX} and stays the same with probability $(1 - w_{XX})$. In Fig. 4a), we begin by encoding the XZ channel and observe simultaneous reduction of both system channels in every iteration. To emphasize that these channels form a DFS, we instead encode only the IY channel in Fig. 4b) and observe that the channels converge in a similar manner. The differences in slopes arise from the weights associated with each channel and do not change the logic of the process. This shows that the partial encoding process, under the XX intrinsic noise, does not create a channel outside the subspace of the system’s channel space.

We now extend our analysis by introducing three noise channels in the form of $\{XX, YY, ZZ\}$ and repeat the partial encoding process for the system channels $\{YI, XZ, ZX, IY\}$. In Fig. 4c), we see a similar simultaneous encoding of the system channels on the quantum computer per iteration. The algorithm truncates at the point when all the system channels have been completely encoded and the residual system channels (y-axis) converge to zero. However, we also observe that the XZ channel is being exceedingly encoded as indicated by the large negative value at the end of the iteration. To mitigate this, we employ our adaptive encoding scheme described in Algorithm 2. In Fig. 4d), we see that the divergences to highly negative values due to this adaptive procedure are successfully tamed. Moreover, we can do better if we define a tolerance below which the iteration can be truncated. This is indicated by the vertical black dotted line and highlights that all channels are encoded within a tolerance of ≈ 0.1 , allowing the iteration to be truncated at the cost of not completely encoding all the channels. The circuits used in all the plots are provided as insets.

B. Benchmarking the algorithm against classical simulations of systems

We benchmark our algorithms with the classically well-understood coherent-dissipative energy transport between molecular aggregates in chemical systems.

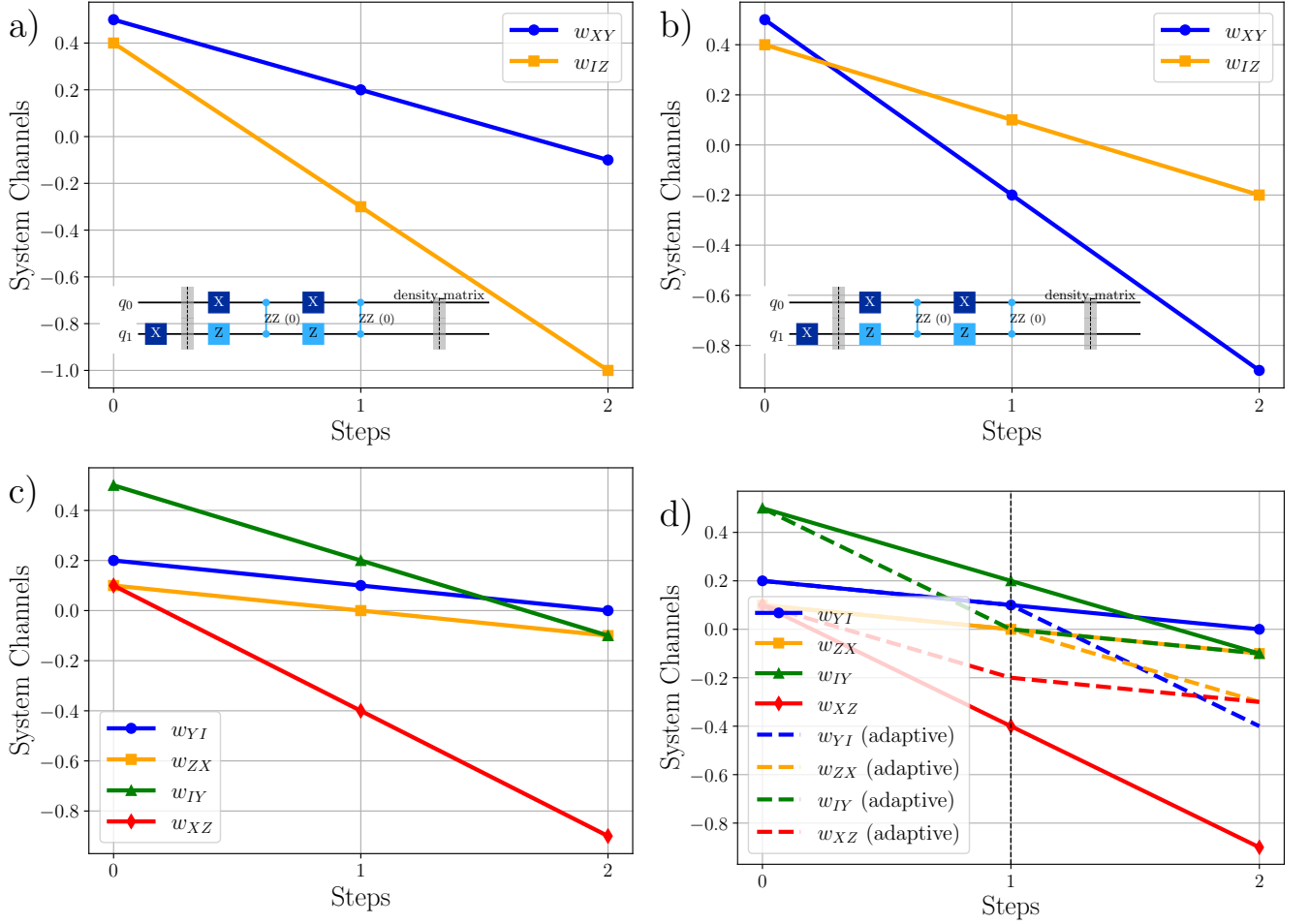


FIG. 4. convergence of the partial encoding algorithms: a) Simultaneous convergence of the residuals for the XY and IY system channels when XY is explicitly encoded (inset). b) Explicitly encoding IY likewise drives simultaneous convergence of both channels. In both a) and b), the residuals of the other 16 channels remain negligible, indicating that under XX intrinsic noise the XY and IY channels map into each other and define a decoherence-free subspace. c) Similar convergence behavior is observed for the set $\{YI, ZX, IY, XZ\}$ in the presence of intrinsic noise $\{XX, YY, ZZ\}$; over-encoding manifests as residuals diverging to large negative values. d) An adaptive scheme that selects which system channel to encode at each step—here choosing XZ and ZX (insets omitted for clarity)—yields improved convergence of residuals toward zero.

These molecular aggregates are usually coupled to a phonon bath that introduces incoherent dynamics in their energy transport. We can model this system as a one-dimensional chain of coupled spins with nearest-neighbor coupling. This is given by the Hamiltonian,

$$H = \frac{\omega_0}{2} \sum_{i=1}^N \sigma_i^z + g \sum_{i=1}^{N-1} (\sigma_i^+ \sigma_{i+1}^- + \sigma_i^- \sigma_{i+1}^+) \quad (18)$$

with open boundary conditions where N is the number of spins. The complete coherent-dissipative energy transport in this model is usually described by the Lindblad master equation in Eq. (2) with the unitary evolution contributed by the Hamiltonian in Eq. (18). However, from the arguments posed in Sec. II, the dynamics of this system can more generally be described by the Pauli noise model in Eq. (5) and we shall resort to this in our

discussion here. In Fig. 5a, we consider a system of two coupled excitons with open system dynamics described by Eq. (16) as shown by solid lines. By partially encoding the system channels onto the noisy quantum circuit, we see that the resulting dynamics (dotted lines) match well with the analytically calculated system dynamics. In each time step of the dynamics, we encode the system channels and allow the residues to converge. This process is repeated over all time steps to ensure that all channels are encoded during each step of the evolution. A similar benchmarking is done in Fig. 5b, where the energy transport between the pair of excitons is $\{ZZ, YY\}$ channels. We see that the dotted lines overlap exactly with the solid lines and demonstrate perfect encoding of the system channels using the intrinsic noise XX . The algorithm also holds for multiple noise channels $\{XX, YY, ZZ\}$. This can be seen in Fig. 5c) where the intrinsic noise

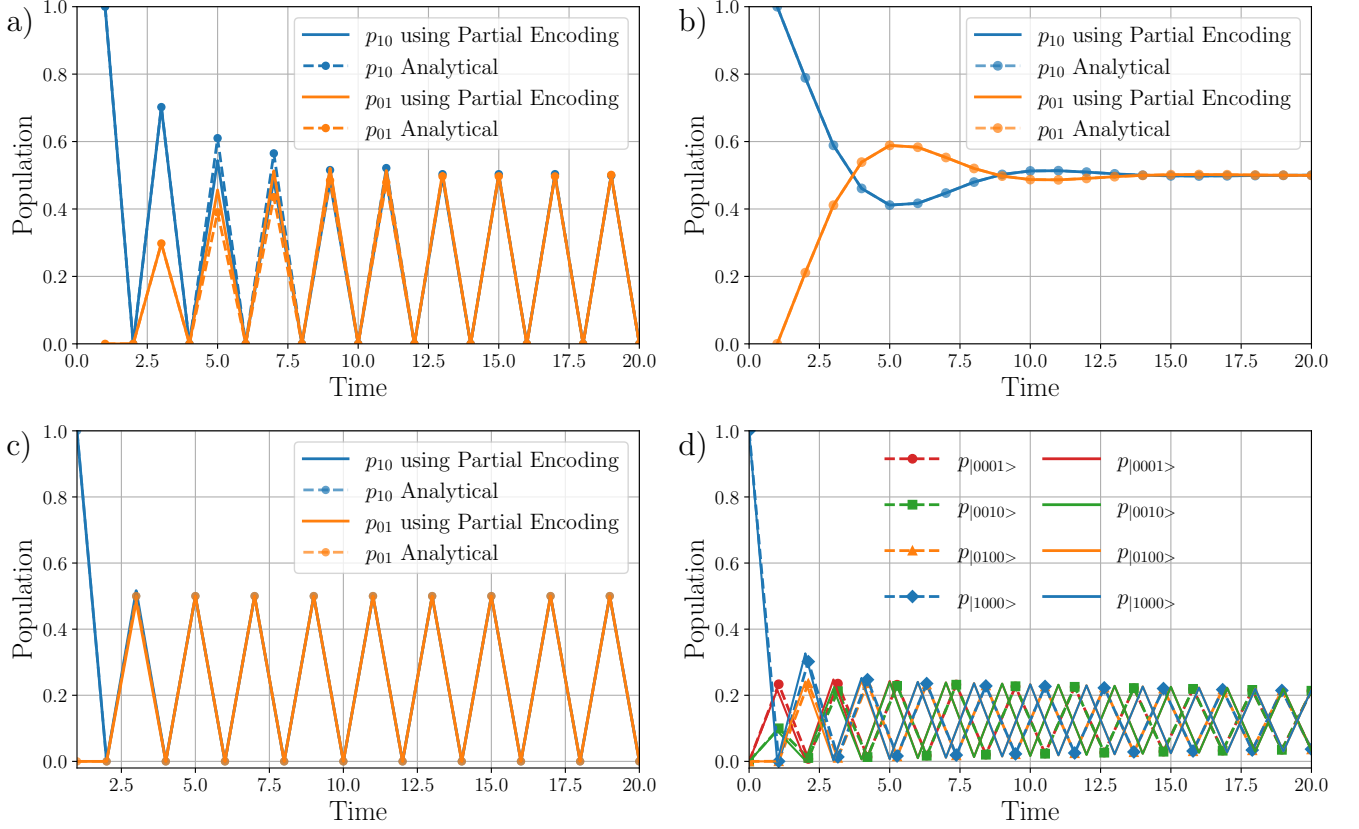


FIG. 5. Benchmarking our algorithm on exciton transport. (a) Two coupled excitons model with $\{XZ, IY\}$ decoherence channels. The dotted lines denote analytical calculations, and the solid lines denote the quantum circuit evolution using partial encoding. (b) shows a similar analysis for $\{ZZ, YY\}$ decoherence channels. In both a) and b), the intrinsic hardware noise channels are $\{XX, II\}$, and analytical and noise-assisted simulations are in close agreement. (c) Here we extend the intrinsic noise $\{XX, YY, ZZ\}$ to encode the $\{XZ, IY, ZX, YI\}$ bath channels of the system. (d) Extension to four nearest-neighbor coupled excitons with system decoherence channels $\{XZZZ, IYIY, IYXZ, XZII\}$ under intrinsic noise $\{XX, II\}$. Our noise-assisted simulations closely match analytical predictions; minor deviations stem from Trotterization of the Hamiltonian's nearest-neighbor terms.

simultaneously encodes $\{XZ, IY, ZX, YI\}$ system channels.

Finally, we extend our system to a chain of multiple excitons with nearest-neighbor coupling. The system channels governing the incoherent energy transport in this model are given as

$$\begin{aligned} \mathcal{E}_{\text{sys}}(\rho) = & w_1 XZZZ\rho XZZZ + w_2 IYIY\rho IYIY \\ & + w_3 IYXZ\rho IYXZ + w_4 XZII\rho XZII. \end{aligned} \quad (19)$$

In Fig. 5d), we see that in the presence of two-qubit bit-flip noise, the algorithm encodes the system channels well and replicates the coherent-dissipative transport dynamics with minor differences. These differences stem from the Trotterization of the various off-diagonal, many-body coupling terms in the Hamiltonian.

Finally, we remark that the system and intrinsic noise channels presented in this work serve merely as examples to demonstrate the algorithms, the formation of clusters, and the braiding structures generated within them.

These channels are not special and can easily be generalized to make the algorithms exhaustive and preserve their rules. More specifically, higher-dimensional sets of intrinsic noise generate higher-dimensional clusters containing multiple braiding structures. The generation of these clusters is guaranteed by the cyclic commutativity of Pauli operators and remains preserved even in highly asymmetric sets of Pauli strings in system and intrinsic noise channels. These properties make our algorithms robust against all kinds of unital noise affecting a quantum processor, and provide a seamless technique to incorporate noise as a computational resource in open quantum system simulations.

IV. SUMMARY

Quantum computers, both today's NISQ and tomorrow's fault-tolerant quantum devices, are constrained by noise: it can corrupt simulations, yield unreliable output

states, or demand a large physical-qubit overhead for error correction. Moreover, fault-tolerant architectures are intrinsically unitary, which poses additional challenges for simulating the nonunitary dynamics of open quantum systems. Rather than suppressing all nonunitary effects to recover perfectly unitary logic, we ask whether intrinsic noise can be leveraged as a computational resource to emulate such dynamics. In this work, we answer this in the affirmative by introducing an ancilla-free technique that constructively encodes a system’s decoherence channels as Pauli strings and averages the device’s inherent noise into the computation, thereby harnessing a resource ubiquitous across physics and chemistry.

We introduce a technique for simulating open-system dynamics that both harnesses hardware noise and reduces qubit requirements compared to existing methods. Our approach partially encodes system dephasing channels as Pauli strings on a quantum circuit. This partial encoding “activates” hardware noise to produce an effective channel that blends the target dynamics with the platform’s intrinsic (dephasing) noise. An iterative procedure then minimizes the mismatch between this effective channel and the desired one, yielding compact circuits that capture open-system behavior without ancillary dilation. We further show that intrinsic noise induces clustering among partially encoded channels via the cyclic commutation structure of Pauli matrices, forming decoherence-free subspaces (DFSs) [72–79] that naturally confine dynamics and can themselves be exploited as resources.

Throughout, we assume a Pauli noise model describing the intrinsic noise and the system’s decoherence chan-

nels. Since this describes unital noise, we plan to explore non-unital noise, such as the T_1 (amplitude damping) channel, in our future work. By turning noise from a liability into an asset, and by relaxing the fidelity demands on logical qubits, our framework reduces qubit- and gate-overhead relative to error-corrected simulations, offers a practical path to studying open-system dynamics on both NISQ and future fault-tolerant hardware, and informs hardware co-design aimed at improving the physical-to-logical qubit ratio for such use cases. Hence, we believe this work represents a substantive step toward early quantum advantage in quantum simulation of open quantum systems.

DATA AVAILABILITY

The source code and data to generate the figures in the paper are available upon request.

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Appendix A: Derivation of Eq. (13)

Following Refs. [82–84], we start by expressing

$$J(\mathcal{E}) = \frac{1}{d} \sum_{i,j} \mathcal{E}(|i\rangle\langle j|) \otimes |i\rangle\langle j|. \quad (\text{A1})$$

Taking the partial trace over the second subsystem $\mathcal{H}_2$, we obtain

$$\begin{aligned} \text{Tr}_2[(\mathbb{I} \otimes \rho^\top)J(\mathcal{E})] &= \frac{1}{d} \sum_{i,j} \mathcal{E}(|i\rangle\langle j|) \langle j|\rho^\top|i\rangle \\ &= \frac{1}{d} \sum_{i,j} \mathcal{E}(|i\rangle\langle j|) \langle i|\rho|j\rangle \\ &= \frac{1}{d} \mathcal{E} \left(\sum_{i,j} \langle i|\rho|j\rangle |i\rangle\langle j| \right) \\ &= \frac{1}{d} \mathcal{E}(\rho). \end{aligned} \quad (\text{A2})$$

Appendix B: Proof of Theorem 1

We now derive upper and lower bounds on the Schatten p -distance between the matrices $(\mathbb{I} \otimes \rho^\top)J(\mathcal{E}_{\text{sys}})$ and $(\mathbb{I} \otimes \rho^\top)J(\mathcal{E}_{\text{eff}})$ for an arbitrary density operator ρ .

We begin with the upper bound. For any ρ , the sub-multiplicativity of the operator norm gives

$$\|(\mathbb{I} \otimes \rho^\top)J(\mathcal{E}_{\text{sys}}) - (\mathbb{I} \otimes \rho^\top)J(\mathcal{E}_{\text{eff}})\|_p^p \leq \|\mathbb{I} \otimes \rho^\top\|_p^p \|J(\mathcal{E}_{\text{sys}}) - J(\mathcal{E}_{\text{eff}})\|_p^p. \quad (\text{B1})$$

From

$$\|\mathbb{I} \otimes \rho^\top\|_p^p = d \text{Tr}[\rho^p], \quad (\text{B2})$$

and the definition of quantum Rényi entropy of order p (≥ 1),

$$S_p(\rho) := \frac{1}{1-p} \ln(\text{Tr}[\rho^p]), \quad (\text{B3})$$

we find

$$\|\mathbb{I} \otimes \rho^\top\|_p^p = d e^{(1-p)S_p(\rho)}. \quad (\text{B4})$$

Hence, for any ρ ,

$$\|(\mathbb{I} \otimes \rho^\top)J(\mathcal{E}_{\text{sys}}) - (\mathbb{I} \otimes \rho^\top)J(\mathcal{E}_{\text{eff}})\|_p^p \leq d e^{(1-p)S_p(\rho)} \|J(\mathcal{E}_{\text{sys}}) - J(\mathcal{E}_{\text{eff}})\|_p^p \leq d \|J(\mathcal{E}_{\text{sys}}) - J(\mathcal{E}_{\text{eff}})\|_p^p, \quad (\text{B5})$$

where we used $p \geq 1$ and $S_p(\rho) \geq 0$, which imply $(1-p)S_p(\rho) \leq 0$.

Next, we derive the lower bound. For any ρ , since

$$\frac{1}{d}\mathcal{E}(\rho) = \text{Tr}_2[(\mathbb{I} \otimes \rho^\top)J(\mathcal{E})], \quad (\text{B6})$$

we have [88]

$$\left\| \frac{1}{d}(\mathcal{E}_{\text{sys}}(\rho) - \mathcal{E}_{\text{eff}}(\rho)) \right\|_p^p = \frac{1}{d^p} \|\mathcal{E}_{\text{sys}}(\rho) - \mathcal{E}_{\text{eff}}(\rho)\|_p^p \leq d^{p-1} \|(\mathbb{I} \otimes \rho^\top)J(\mathcal{E}_{\text{sys}}) - (\mathbb{I} \otimes \rho^\top)J(\mathcal{E}_{\text{eff}})\|_p^p. \quad (\text{B7})$$

Therefore, for any ρ ,

$$\frac{1}{d^{2p-1}} \|\mathcal{E}_{\text{sys}}(\rho) - \mathcal{E}_{\text{eff}}(\rho)\|_p^p \leq \|(\mathbb{I} \otimes \rho^\top)J(\mathcal{E}_{\text{sys}}) - (\mathbb{I} \otimes \rho^\top)J(\mathcal{E}_{\text{eff}})\|_p^p. \quad (\text{B8})$$

Finally, combining Eqs. (B5) and (B8), we obtain

$$0 \leq \|\mathcal{E}_{\text{sys}}(\rho) - \mathcal{E}_{\text{eff}}(\rho)\|_p \leq d^2 \|J(\mathcal{E}_{\text{sys}}) - J(\mathcal{E}_{\text{eff}})\|_p \quad (\forall \rho). \quad (\text{B9})$$