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Symmetry criteria for quantum simulability of effective interactions

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What can one do with a given tunable quantum device? We provide complete symmetry criteria deciding whether some effective target interaction(s) can be simulated by a set of given interactions. Symmetries lead to a better understanding of simulation and permit a reasoning beyond the limitations of the usual explicit Lie closure. Conserved quantities induced by symmetries pave the way to a resource theory for simulability. On a general level, one can now decide equality for any pair of compact Lie algebras just given by their generators without determining the algebras explicitly. Several physical examples are illustrated, including entanglement invariants, the relation to unitary gate membership problems, as well as the central-spin model.

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I. INTRODUCTION

Thanks to impressive progress on the experimental side, many small- and medium-scale quantum devices are now ready for applications ranging from quantum metrology [1–4] to quantum simulation [5–9]. With quantum information processing as one of the driving but long-term goals (e.g., [10–12]), one of the pressing questions is, what can one do with these devices *now*? This problem clearly falls into the remit of *quantum systems and control engineering*, an area naturally receiving increased interest [13–15] both experimentally and theoretically.

Control theory offers a well-known characterization of the operations that a quantum device is capable of on *Lie-algebraic* grounds [14,16–21]. In this work, we simplify the question to the *Hamiltonian membership problem* of (finite-dimensional) quantum simulation. It amounts to deciding, for a set of *given control interactions* $\mathcal{P}$, whether a set of *effective target interactions* $\mathcal{Q}$ can be simulated—without having to establish controllability via nested (and hence tedious) commutator calculations for the so-called Lie closure. Our results reduce the Hamiltonian membership problem to the straightforward solution of homogeneous linear equations.

In the setting of the controlled Schrödinger equation [22] (taken as a bilinear control system [17,23])

$$\frac{d}{dt}U(t) = \left[-iH_1 + \sum_{\nu=2}^{p} -iu_\nu(t)H_\nu \right]U(t), \tag{1}$$

we ask whether the given set $\mathcal{P} := \{iH_1, \ldots, iH_p\}$ of interactions (which may include a drift term) generates an effective interaction iH_{p+1} or, more generally, any interaction from a set $\mathcal{Q} := \{iH_{p+1}, \ldots, iH_q\}$ assuming all H_ν are represented by Hermitian matrices henceforth. If so, then for *every* evolution time $\tau > 0$ of a *simulated interaction* $iH_k \in \mathcal{Q}$, there is a solution $U(t)$ of the *simulating system* (1) for $0 \leqslant t \leqslant \theta$ and controls $u_\nu(t)$ such that $\mathcal{P}$ generates a unitary $U(\theta) = \exp(-i\tau H_k)$ in the simulation time θ starting from the identity at $t = 0$ [6,24–31]. In this sense, Hamiltonian simulation of a particular Hamiltonian H_k can be considered as an infinitesimal version of creating a particular unitary gate. It also generalizes the universality (or full controllability) question of whether *all* Hamiltonians can be simulated (or, equivalently, whether *all* unitary gates can be obtained) [19,28,32–41]. In the context of gates, a familiar elementary example is that all unitary gates in an n-qubit system can be obtained [32] by combining local gates with CNOT gates. However, the approach of the pioneering age of decomposing every target gate into a sequence of CNOT and local gates is, in practice, all too often imprecise or slow. So implementing gates or simulating Hamiltonians with high fidelity rather asks for optimal control techniques, as explained in a recent road map [42]. As a precondition, here we step back to the Hamiltonian level and give criteria for simulability and controllability.

II. MAIN IDEA

We solve the decision problems of simulability (and controllability) by just analyzing the symmetries of the Hamiltonians of given setups. We show that this decision requires considering both *linear and quadratic symmetries*, where linear symmetries of a Hamiltonian H commute with H, while *quadratic symmetries* of H are those commuting with the tensor square $(iH \otimes \mathbb{1} + \mathbb{1} \otimes iH)$. The term quadratic symmetry is motivated, since the tensor square generates $U \otimes U$ just as iH generates the unitary U.

More precisely, our goal is to get a symmetry-based understanding of how a set $\mathcal{P}$ of available interactions can simulate a set $\mathcal{Q}$ of desired effective quantum interactions in the sense that the Lie closures coincide, i.e., $\langle \mathcal{P} \rangle = \langle \mathcal{P} \cup \mathcal{Q} \rangle$. We circumvent brute-force calculation of the Lie closure not only because high-order commutators can entail a significant growth in the appearing matrix entries and may lead to instabilities in numerical computations, but first and foremost because it provides no deeper insight into the problem. Our symmetry analysis leads to a much more systematic understanding of Hamiltonian simulation and quantum system dynamics in general. It provides a powerful argument to decide under which conditions a desired Hamiltonian can, in fact, be simulated or, in turn, which explicit simulations or computations are impossible in a given experimental setup.

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Let us summarize our line of thought: As shorthand, let the *linear symmetries* of $\mathcal{P}$ (analogously for any set of matrices) be expressed via the *commutant* $\mathcal{P}'$, which consists of all matrices $S \in \mathbb{C}^{d\times d}$ that commute (i.e., $[S,iH_\nu]=0$) with each element $iH_\nu \in \mathbb{C}^{d\times d}$ of $\mathcal{P}$ [43]. Obviously, for $\mathcal{Q}$ to be simulable by $\mathcal{P}$, it is necessary that $\mathcal{Q}$ may not break but rather has to inherit the symmetries of $\mathcal{P}$, so $\dim[\mathcal{P}'] = \dim[(\mathcal{P}\cup\mathcal{Q})']$. However, a complete symmetry characterization is nontrivial. It rather requires the following two steps: The first is to introduce *quadratic* symmetries [19] as those linear symmetries of the system artificially doubled by the *tensor square* $\mathcal{P}^{\otimes 2} := \{iH_\nu\otimes\mathbb{1}_d+\mathbb{1}_d\otimes iH_\nu \text{ for } \nu \in \{1,\ldots,p\}\}$. It defines the *quadratic symmetries* by its commutant $\mathcal{P}^{(2)} := (\mathcal{P}^{\otimes 2})'$. Second, let $\mathcal{C}$ denote the center [44] of the commutant $(\mathcal{P}\cup\mathcal{Q})'$ and consider the central projections of $\mathcal{P}$ and $\mathcal{P}\cup\mathcal{Q}$ onto $\mathcal{C}$. With these stipulations, we summarize our main result:

Main result (see Result 1 below). The given interactions $\mathcal{P}$ simulate the desired interactions $\mathcal{Q}$ in the sense $\langle\mathcal{P}\rangle = \langle\mathcal{P}\cup\mathcal{Q}\rangle$ if and only if $\mathcal{P}$ and $\mathcal{Q}$ share the same *quadratic* symmetries (i.e., $\dim[\mathcal{P}^{(2)}] = \dim[(\mathcal{P}\cup\mathcal{Q})^{(2)}]$) [condition (A)] and the central projections of $\mathcal{P}$ and $\mathcal{P}\cup\mathcal{Q}$ onto $\mathcal{C}$ are of the same rank [condition (B)].

Let us emphasize that our approach goes beyond the ubiquitous use of linear symmetries in physics, since linear symmetries provide only an incomplete picture of Hamiltonian simulation. The application of higher symmetries is the key here. It is interesting to note that essentially only the quadratic symmetries (and no higher ones) in condition (A) are necessary to characterize the dynamics of a quantum system. One obtains a complete description together with the auxiliary condition (B).

Some remarks also summarizing known approaches are in order. The quadratic symmetries are stronger than the linear ones; actually they include them and thus condition (A) implies that the linear symmetries also agree. Example 1 below illustrates why matching the linear symmetries does not suffice to ensure simulability. As shown in a companion paper [45], one can decide if a subalgebra $\mathfrak{h} \subseteq \mathfrak{g}$ of a compact semisimple Lie algebra $\mathfrak{g}$ actually fulfills $\mathfrak{h} = \mathfrak{g}$ (e.g., $\langle\mathcal{P}\rangle = \langle\mathcal{P}\cup\mathcal{Q}\rangle$) just by analyzing quadratic symmetries. But Example 2 elucidates why condition (A) alone does not, in the general compact case, imply simulability. Only after fixing the central projections by condition (B) do the quadratic symmetries decide simulability.

On a much more general scale, condition (B) closes the gap to completely characterizing equality in $\mathfrak{h} \subseteq \mathfrak{g}$ now for *all compact Lie algebras* (generated by skew-Hermitian interactions) beyond the semisimple ones of [45]. Simplifying within the Lie-algebraic frame, our symmetry approach to decide simulability and the membership $\mathcal{Q} \subseteq \langle\mathcal{P}\rangle$ can thus be seen as a major step beyond the well-established Lie-algebra rank condition [14,16,17] and beyond the limited first use of quadratic symmetries to establish full controllability in [19].

III. SYMMETRIES

In this section, we elaborate our method and establish necessary and sufficient conditions for Hamiltonian simulation to arrive at Result 1 below. We also describe important properties of linear and quadratic symmetries and discuss two illustrating examples. Example 1 highlights the importance of quadratic symmetries for deciding Hamiltonian simulation and their relevance for entanglement invariants. The necessity for the auxiliary condition (B) is made evident in Example 2.

The linear symmetries of $\mathcal{M} \subseteq \mathbb{C}^{d\times d}$ are identified [19] with the commutant $\mathcal{M}'$ given as

$$\mathcal{M}' := \{S \in \mathbb{C}^{d\times d} \text{ such that } [S,M]=0 \text{ for all } M \in \mathcal{M}\}.$$

The commutant includes all complex multiples of the identity $\mathbb{1}_d$ and it forms a vector space of dimension $\dim(\mathcal{M}')$. A smaller set of matrices typically shows *more* symmetries, i.e., for $\mathcal{M}_1 \subseteq \mathcal{M}_2$, one has $\mathcal{M}_1' \supseteq \mathcal{M}_2'$ and $\mathcal{M}_1' = \mathcal{M}_2'$ iff $\dim(\mathcal{M}_1') = \dim(\mathcal{M}_2')$. By Jacobi's identity (i.e., $[S,[M_1,M_2]] = [[M_2,S],M_1] + [[S,M_1],M_2]$), any symmetry S that commutes with both M_1 and M_2 also commutes with their commutator $[M_1,M_2]$. So, $\mathcal{M}$ and the Lie algebra $\langle\mathcal{M}\rangle$ it generates have the same commutant: $\mathcal{M}_1' = \mathcal{M}_2'$ if $\langle\mathcal{M}_1\rangle = \langle\mathcal{M}_2\rangle$.

In our context, this implies that iH_{p+1} cannot be simulated by $\mathcal{P}$ unless $\mathcal{P}' = (\mathcal{P}\cup\{iH_{p+1}\})'$, i.e., coinciding symmetries are a necessary but not sufficient condition. This is because the converse does not hold as the following basic example illustrates:

Example 1. The pair interaction $iH_{zz} := iZ_1Z_2$ cannot be simulated by the local interactions $\mathcal{P} = \{iX_1,iY_1,iX_2,iY_2\}$ of a two-qubit system [46] in spite of coinciding (trivial) commutants $\mathcal{P}' = (\mathcal{P}\cup\{iH_{zz}\})' = \mathbb{C}\mathbb{1}_4$.

Thus, we further discuss *quadratic symmetries* [19] defined by the commutant to the tensor square [47],

$$\mathcal{M}^{(2)} := (\mathcal{M}^{\otimes 2})' = \{S \in \mathbb{C}^{d^2\times d^2} \text{ such that}$$
$$[S, M\otimes\mathbb{1}_d+\mathbb{1}_d\otimes M] = 0 \text{ for all } M \in \mathcal{M} \subseteq \mathbb{C}^{d\times d}\}.$$

The tensor-square commutant always contains (the subspace spanned by) the identity $\mathbb{1}_{d^2}$ and the SWAP or commutation matrix $K_{d,d}$ [48]. Also, the quadratic symmetries include all linear ones, i.e., $S_1\otimes\mathbb{1}_d+\mathbb{1}_d\otimes S_1 \in \mathcal{M}^{(2)}$ for $S_1 \in \mathcal{M}'$. And by Jacobi's identity [51], one finds $(\mathcal{M}_1)^{(2)} = (\mathcal{M}_2)^{(2)}$ if $\langle\mathcal{M}_1\rangle = \langle\mathcal{M}_2\rangle$. As above, in our context this implies that iH_{p+1} cannot be simulated by $\mathcal{P}$ unless $\mathcal{P}^{(2)} = (\mathcal{P}\cup\{iH_{p+1}\})^{(2)}$ holds.

Example 1 (completion). The relevant tensor-square commutants have different dimensions $\dim[\mathcal{P}^{(2)}] = 4$ and $\dim[(\mathcal{P}\cup\{iH_{zz}\})^{(2)}] = 2$, so iH_{zz} cannot be simulated. Naturally, $(\mathcal{P}\cup\{iH_{zz}\})^{(2)}$ contains $\mathbb{1}_{16}$ and the commutation matrix $K_{4,4}$, which is related to the joint permutation (1,3)(2,4) of tensor components in $\mathbb{C}^{16\times 16}$, while $\mathcal{P}^{(2)}$ contains two additional quadratic symmetries related to the separate permutations (1,3) and (2,4); see Fig. 1. Evidently, the local interactions of $\mathcal{P}$ cannot generate entanglement. Hence, a quadratic symmetry in $\mathcal{P}^{(2)}$ has a physical interpretation as an entanglement invariant. Indeed, the

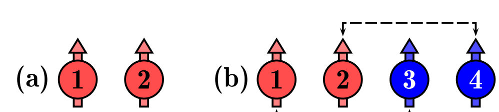

FIG. 1. (Color online) Visualization of Example 1. (a) No linear symmetries besides the identity exist for both the fully controllable system and the local interactions. (b) The doubled system reveals nontrivial quadratic symmetries corresponding to separate permutations (1,3) and (2,4).

concurrence [52] of a two-qubit pure state $|\psi\rangle$ can be defined as $[\langle\psi|\langle\psi|\mathbb{1}_{16}-M_{(1,3)}-M_{(2,4)}+M_{(1,3)(2,4)}|\psi\rangle|\psi\rangle]^{1/2}/2$ [53–56], where the matrix M_p is defined by the permutation p. Any quadratic symmetry $S \in \mathcal{P}^{(2)}$ relates to a degree-two polynomial invariant $\mathrm{Tr}[\rho\otimes\rho\, S]$ in the entries of the density matrix ρ [57].

Remarkably, symmetries beyond quadratic ones (i.e., those of the tensor square) are not required for a necessary and sufficient condition for simulability [58]. Concerning the tensor-square commutant, we build on two important classification-free results of [45] for compact Lie algebras [59,60] (as generated by skew-Hermitian matrices iH_ν): For $\langle\mathcal{P}\cup\mathcal{Q}\rangle$ being *semisimple* (and compact), Ref. [45] first shows that $\langle\mathcal{P}\rangle = \langle\mathcal{P}\cup\mathcal{Q}\rangle$ holds if and only if $\dim[\mathcal{P}^{(2)}] = \dim[(\mathcal{P}\cup\mathcal{Q})^{(2)}]$. Beyond the semisimple case, any compact Lie algebra $\mathfrak{g}$ can be uniquely decomposed as $\mathfrak{g} = \mathfrak{s}\oplus\mathfrak{c}$ into its semisimple part $\mathfrak{s}$ and its center $\mathfrak{c}$ (where $\mathfrak{s} := [\mathfrak{g},\mathfrak{g}]$ and $[\mathfrak{g},\mathfrak{c}] = 0$ [44]). So Ref. [45] secondly verifies that the semisimple parts of $\langle\mathcal{P}\rangle$ and $\langle\mathcal{P}\cup\mathcal{Q}\rangle$ have to agree if $\dim[\mathcal{P}^{(2)}] = \dim[(\mathcal{P}\cup\mathcal{Q})^{(2)}]$. When generalizing from semisimple to arbitrary compact Lie algebras, the equality of the two tensor-square commutants implies that $\langle\mathcal{P}\rangle$ and $\langle\mathcal{P}\cup\mathcal{Q}\rangle$ agree—except for the central elements (commuting with all the other ones). These commuting interactions require condition (B) to fix the central projection, thus resulting in the following complete characterization:

Result 1. Consider two sets $\mathcal{P} := \{iH_1,\dots,iH_p\}$ and $\mathcal{Q} := \{iH_{p+1},\dots,iH_q\}$ of (skew-Hermitian) interactions, and let C_α denote elements of a linear basis spanning the center $\mathcal{C}$ of the commutant $(\mathcal{P}\cup\mathcal{Q})'$. For the central projections, define the matrix T by its entries $T_{\alpha\beta} := \mathrm{Tr}(C_\alpha^\dagger iH_\beta)$ for $1 \leqslant \alpha \leqslant \dim(\mathcal{C})$ and $1 \leqslant \beta \leqslant q$, as well as $\widetilde{T}$ by $\widetilde{T}_{\alpha\beta} := \mathrm{Tr}(C_\alpha^\dagger iH_\beta)$ for $1 \leqslant \beta \leqslant p$. Then, $\mathcal{P}$ simulates $\mathcal{Q}$ in the sense $\langle\mathcal{P}\rangle = \langle\mathcal{P}\cup\mathcal{Q}\rangle$, if and only if both conditions (A) $\dim[\mathcal{P}^{(2)}] = \dim[(\mathcal{P}\cup\mathcal{Q})^{(2)}]$ and (B) $\mathrm{rank}(\widetilde{T}) = \mathrm{rank}(T)$ are fulfilled.

Condition (B) of Result 1 is a basic linear-algebra test solely based on linear symmetries. Each of the matrices $\widetilde{T}$ and T depends on both $\mathcal{P}$ and $\mathcal{Q}$. In Example 1, iH_{zz} could not be generated as condition (A) is not satisfied. Before proving Result 1, the following example provides a helpful illustration of condition (B):

Example 2. In a two-qubit system, consider a dipole coupling combined with a tilted magnetic field, i.e., $\mathcal{P} := \{i(2Z_1Z_2-X_1X_2-Y_1Y_2), i(X_1-Y_1+X_2-Y_2)\}$. We investigate whether a Heisenberg-type interaction of the form $\mathcal{Q}_a := \{i(X_1X_2+Y_1Y_2+Z_1Z_2)\}$ or one particular interaction of pairing type (i.e., $\mathcal{Q}_b := \{i(X_1Z_2+Z_1X_2+Y_1Z_2+Z_1Y_2)\}$) can be simulated. Condition (A) is satisfied in both cases as the quadratic symmetries of $\mathcal{P}$, $\mathcal{P}\cup\mathcal{Q}_a$, and $\mathcal{P}\cup\mathcal{Q}_b$ all coincide (there are 16 of them). The three linear symmetries also agree. Moreover, with the mutually commuting operators

$$\begin{pmatrix}1&0&0&0\\0&1&0&0\\0&0&1&0\\0&0&0&1\end{pmatrix}, \quad \begin{pmatrix}1&0&0&0\\0&0&1&0\\0&1&0&0\\0&0&0&1\end{pmatrix}, \quad \text{and}$$

$$\begin{pmatrix}0&0&0&1\\0&0&-i&0\\0&-i&0&0\\-1&0&0&0\end{pmatrix}$$

forming a basis of the commutants $\mathcal{P}' = (\mathcal{P}\cup\mathcal{Q}_a)' = (\mathcal{P}\cup\mathcal{Q}_b)'$, they also span the (three-dimensional) center $\mathcal{C}$. For the central projections, one thus gets the matrices

$$T_a = \begin{pmatrix}0&0&0\\0&0&6i\\4&0&-4\end{pmatrix}, \quad T_b = \begin{pmatrix}0&0&0\\0&0&0\\4&0&0\end{pmatrix}, \quad \text{and}$$

$$\widetilde{T}_a = \widetilde{T}_b = \begin{pmatrix}0&0\\0&0\\4&0\end{pmatrix}.$$

Condition (B) reveals $\mathrm{rank}(\widetilde{T}_a) \neq \mathrm{rank}(T_a)$, $\mathrm{rank}(\widetilde{T}_b) = \mathrm{rank}(T_b)$, so $\mathcal{Q}_a$ cannot be simulated by $\mathcal{P}$, while $\mathcal{Q}_b$ can. Note the isomorphy types of $\langle\mathcal{P}\rangle$, $\langle\mathcal{P}\cup\mathcal{Q}_a\rangle$, and $\langle\mathcal{P}\cup\mathcal{Q}_b\rangle$ are $\mathfrak{su}(2)\oplus\mathfrak{u}(1)$, $\mathfrak{su}(2)\oplus\mathfrak{u}(1)\oplus\mathfrak{u}(1)$, and $\mathfrak{su}(2)\oplus\mathfrak{u}(1)$.

Proof of Result 1. Decompose the compact Lie algebras $\langle\mathcal{P}\rangle$ and $\langle\mathcal{P}\cup\mathcal{Q}\rangle$ into their semisimple parts and centers. If condition (A) holds, the semisimple parts coincide, $\langle\mathcal{P}\rangle = \mathfrak{s} + \mathfrak{c}_\mathcal{P}$ and $\langle\mathcal{P}\cup\mathcal{Q}\rangle = \mathfrak{s} + \mathfrak{c}_{\mathcal{P}\cup\mathcal{Q}}$ with $\mathfrak{c}_\mathcal{P} \subseteq \mathfrak{c}_{\mathcal{P}\cup\mathcal{Q}}$. Take the unique decomposition $iH_\ell = iH_\ell^\mathfrak{s} + iH_\ell^\mathfrak{c}$ with $iH_\ell^\mathfrak{s} \in \mathfrak{s}$ and $iH_\ell^\mathfrak{c} \in \mathfrak{c}_{\mathcal{P}\cup\mathcal{Q}}$. Since $[iH_n,iH_m] \in \mathfrak{s}$, the real-linear span of $\{iH_1^\mathfrak{c},\dots,iH_p^\mathfrak{c}\}$ agrees with $\mathfrak{c}_\mathcal{P}$, while the one of $\{iH_1^\mathfrak{c},\dots,iH_q^\mathfrak{c}\}$ equals $\mathfrak{c}_{\mathcal{P}\cup\mathcal{Q}}$. It follows that $\mathfrak{c}_\mathcal{P} = \mathfrak{c}_{\mathcal{P}\cup\mathcal{Q}}$ iff the dimensions of the two real-linear spans agree; this in turn is equivalent to the dimensions of the two complex-linear spans being equal because all relevant Lie algebras are compact (see Corollary 1 of Theorem 1 in Chapter IX, Sec. 3.3 of [60]).

The center $\mathfrak{c}$ of a compact Lie algebra $\mathfrak{g}$ lies within the center $\mathcal{C}$ of its matrix commutant $\mathfrak{g}'$: $[c,g] = 0$ for $c \in \mathfrak{c}$, $g \in \mathfrak{g}$ implies $\mathfrak{c} \subseteq \mathfrak{g}'$; likewise, $[s,c] = 0$ for $s \in \mathfrak{g}'$ shows that $\mathfrak{c} \subseteq \mathcal{C}$. Given the basis $\{C_\alpha\}$ of $\mathcal{C}$, introduce its dual basis $\{B_\alpha\}$ with respect to the Hilbert-Schmidt scalar product via $\mathrm{Tr}(C_\alpha^\dagger B_\beta) = \delta_{\alpha,\beta}$. So any $C \in \mathcal{C}$ can be written as $C = \sum_\alpha \mathrm{Tr}(C_\alpha^\dagger C)\, B_\alpha$. Define the matrix K entrywise by $K_{\alpha\beta} := \mathrm{Tr}(C_\alpha^\dagger iH_\beta^\mathfrak{c})$ for $1 \leqslant \alpha \leqslant \dim(\mathcal{C})$ and $1 \leqslant \beta \leqslant q$, and similarly $\widetilde{K}$ by $\widetilde{K}_{\alpha\beta} := \mathrm{Tr}(C_\alpha^\dagger iH_\beta^\mathfrak{c})$ for $1 \leqslant \beta \leqslant p$. Hence the dimension of $\mathfrak{c}_{\mathcal{P}\cup\mathcal{Q}}$ agrees with the rank of K, and the dimension of $\mathfrak{c}_\mathcal{P}$ equals the rank of $\widetilde{K}$.

Now, for any $b \in \mathfrak{s}$, there are two elements $b_1,b_2 \in \mathfrak{s}$ with $b = [b_1,b_2]$ (Chapter I, Sec. 6.4, Proposition 5 of [59]). Thus, $\mathrm{Tr}(C_\alpha b) = \mathrm{Tr}(C_\alpha[b_1,b_2]) = \mathrm{Tr}(C_\alpha b_1 b_2) - \mathrm{Tr}(C_\alpha b_2 b_1) = \mathrm{Tr}(C_\alpha b_1 b_2) - \mathrm{Tr}(b_2 C_\alpha b_1) = \mathrm{Tr}(C_\alpha b_1 b_2) - \mathrm{Tr}(C_\alpha b_1 b_2) = 0$, where the third equality follows as $C_\alpha \in \mathcal{C}$ and b_2 commute, and cyclic permutations in the trace imply the fourth equality. Moreover, $\mathrm{Tr}(C_\alpha^\dagger b) = -\mathrm{Tr}(C_\alpha^\dagger b^\dagger) = -\overline{\mathrm{Tr}(C_\alpha b)} = 0$. Hence, $\mathrm{Tr}(C_\alpha^\dagger iH_\beta) = \mathrm{Tr}(C_\alpha^\dagger iH_\beta^\mathfrak{c})$, which implies $T = K$ and $\widetilde{T} = \widetilde{K}$. In summary, $\mathfrak{c}_\mathcal{P} = \mathfrak{c}_{\mathcal{P}\cup\mathcal{Q}}$ iff the ranks of T and $\widetilde{T}$ agree, which proves Result 1. ■

IV. ALGORITHMICS AND BEYOND

Both linear and quadratic symmetries can readily be computed by standard linear algebra: Linear symmetries $S \in \mathbb{C}^{d\times d}$ are determined by the commutant and can be obtained by solving the linear equations $(\mathbb{1}_d\otimes M - M^t\otimes\mathbb{1}_d)\,\mathrm{vec}(S) = 0$ jointly for all $M \in \mathcal{M} \subseteq \mathbb{C}^{d\times d}$ [19,50]. Here, $\mathrm{vec}(S)$ is a column vector of length d^2 stacking all columns of S [49]. The dimension of the solution is d^2-r, where r denotes the rank of the matrix formed by vertically stacking the matrices $\mathbb{1}_d\otimes M - M^t\otimes\mathbb{1}_d$. Likewise, the quadratic symmetries $S \in \mathbb{C}^{d^2\times d^2}$ (given

TABLE I. Central-spin model of Example 3: number n of spins, Lie dimensions $\dim(\langle\mathcal{P}\rangle) = \dim(\langle\mathcal{P}\cup\mathcal{Q}\rangle)$, the isomorphy type, dimensions of quadratic and linear symmetries (i.e., $\dim[\mathcal{P}^{(2)}] = \dim[(\mathcal{P}\cup\mathcal{Q})^{(2)}]$ and $\dim[\mathcal{P}'] = \dim[(\mathcal{P}\cup\mathcal{Q})']$), and ranks of the central projections [i.e., $\mathrm{rank}(\widetilde{T}) = \mathrm{rank}(T)$].

n	Lie dimensions	Isomorphy type	No. of symmetries: Quadratic	No. of symmetries: Linear	Rank of central projections
Case (a): $J_k = 1$					
2	15	$\mathfrak{su}(4)$	2	1	0
3	38	$\mathfrak{su}(2)\oplus\mathfrak{su}(6)$	8	2	0
4	78	$\mathfrak{su}(4)\oplus\mathfrak{su}(8)$	50	5	0
5	137	$\mathfrak{su}(2)\oplus\mathfrak{su}(6)\oplus\mathfrak{su}(10)$	392	14	0
6	221	$\mathfrak{su}(4)\oplus\mathfrak{su}(8)\oplus\mathfrak{su}(12)$	3528	42	0
Case (b): $J_k = 2$ for even k, and $J_k = 1$ otherwise					
2	15	$\mathfrak{su}(4)$	2	1	0
3	63	$\mathfrak{su}(8)$	2	1	0
4	158	$\mathfrak{su}(4)\oplus\mathfrak{su}(12)$	8	2	0
5	396	$\mathfrak{su}(2)\oplus\mathfrak{su}(6)\oplus\mathfrak{su}(6)\oplus\mathfrak{su}(18)$	32	4	0
6	796	$\mathfrak{su}(4)\oplus\mathfrak{su}(8)\oplus\mathfrak{su}(12)\oplus\mathfrak{su}(24)$	200	10	0

by the tensor-square commutant) just amount to solving $[\mathbb{1}_{d^2}\otimes(M\otimes\mathbb{1}_d+\mathbb{1}_d\otimes M)-(M\otimes\mathbb{1}_d+\mathbb{1}_d\otimes M)^t\otimes\mathbb{1}_{d^2}]\,\mathrm{vec}(S)=0$ jointly for all $M\in\mathcal{M}$. The preceding discussion explains how to explicitly determine linear and quadratic symmetries. This allows us to test condition (A) (i.e., $\dim[\mathcal{P}^{(2)}] = \dim[(\mathcal{P}\cup\mathcal{Q})^{(2)}]$) by comparing the dimensions of the quadratic symmetries for $\mathcal{P}$ and $\mathcal{P}\cup\mathcal{Q}$.

As the commutant $(\mathcal{P}\cup\mathcal{Q})'$ represents the linear symmetries of $\mathcal{P}\cup\mathcal{Q}$, its center $\mathcal{C}$ is readily obtained by solving the linear equations $(\mathbb{1}_d\otimes M-M^t\otimes\mathbb{1}_d)\,\mathrm{vec}(C)=0$ and $(\mathbb{1}_d\otimes S-S^t\otimes\mathbb{1}_d)\,\mathrm{vec}(C)=0$ jointly with M extending over all $M\in\mathcal{P}\cup\mathcal{Q}$ and S over all $S\in(\mathcal{P}\cup\mathcal{Q})'$. Solving for C yields a basis C_α of the center $\mathcal{C}$, and one can determine the matrices T and $\widetilde{T}$ as $T_{\alpha\beta}=\mathrm{Tr}(C_\alpha^\dagger iH_\beta)$ for $1\leqslant\alpha\leqslant\dim(\mathcal{C})$ and $1\leqslant\beta\leqslant q$, as well as $\widetilde{T}_{\alpha\beta}=\mathrm{Tr}(C_\alpha^\dagger iH_\beta)$ for $1\leqslant\beta\leqslant p$. Since condition (B) is given by $\mathrm{rank}(\widetilde{T})=\mathrm{rank}(T)$, it can easily be tested by elementary linear-algebra computations comparing the ranks of $\tilde{T}$ and T. To sum up, Result 1 reduces the Hamiltonian membership problem to straightforward solutions of homogeneous linear equations.

Example 3 (*central-spin model*). Consider a central spin interacting with $n-1$ surrounding spins via a star-shaped coupling graph (where the surrounding spins may be taken as uncontrolled spin bath) [61–63]. The interactions amount to a drift term (tunneling plus coupling) and just a local Z control on the central spin, $\mathcal{P}:=\{iX_1+i\sum_{k=2}^n J_k(X_1X_k+Y_1Y_k+Z_1Z_k),\, iZ_1\}$. We ask whether the central spin can be fully controlled, i.e., if $\mathcal{Q}:=\{iX_1\}$ can be simulated. Depending on the interaction strengths $J_k\in\mathbb{R}$ for $k\geqslant 2$, different cases are possible: (a) with $J_k=1$ and (b) with $J_k=2$ for even k, and $J_k=1$ otherwise.

Computational results for the central-spin model have been obtained using exact arithmetic [64] for a moderate number of spins, as detailed in Table I. These results vary significantly for different coupling strengths J_k. But our approach for deciding simulability allows for analytic reasoning even beyond specific choices of J_k. For Hamiltonian simulation, it thus provides a powerful technique to analyze and understand the dynamics of general quantum systems. This even holds if the symmetries cannot be calculated explicitly. Showcases for the strength of explicit symmetries are given in Examples 1–3, while Example 3 also makes use of symmetries implicitly (in parts where they cannot be calculated explicitly) via the proofs of the Appendix A. These proofs motivate the following:

Conjecture. In the central-spin model of Example 3, the central spin is fully controllable for a finite number of spins and any choice of J_k (i.e., iX_1 can be simulated, and the surrounding spins can be uncoupled by applying the control).

V. DISCUSSION

Similar to the Hamiltonian membership problem for interactions solved here, one may address membership for groups, e.g., (i) in the (prototypical) discrete case, (ii) in connected compact Lie groups, and (iii) in nonconnected compact groups including finite groups.

In *discrete groups* (i), asking the question (a) if $\hat{\mathcal{Q}}=\{U_{p+1}\}$ is (exactly) contained in the group generated by the unitaries $\hat{\mathcal{P}}=\{U_1,\dots,U_p\}$ is undecidable for $SU(N)$ (at least for $N\geqslant 4$) [65]. Yet the question (b) of approximate universality [66,67], i.e., if all unitaries in $SU(N)$ can be approximated, is decidable [65,68] by comparing the matrix algebra generated by elements $\bar{U}_\nu\otimes U_\nu$ for $U_\nu\in\hat{\mathcal{P}}$ with its equivalent for $SU(N)$ (plus other conditions). Still, the tedious algebra closure is needed, similar to the Lie closure. Question (b) is equivalent to comparing the *topological closure* of the group generated by $\hat{\mathcal{P}}$ to $SU(N)$ and thus leads to (ii).

In *continuous groups* (ii), Result 1 applies to decide if two connected, compact Lie groups (given by their infinitesimal generators) are equal:

Result 2. Given two sets $\mathcal{P}$ and $\mathcal{Q}$ of (skew-Hermitian) interactions, the elements of $\mathcal{P}$ simulate the ones of $\mathcal{Q}$ *and vice versa* iff both $\langle\mathcal{P}\rangle=\langle\mathcal{P}\cup\mathcal{Q}\rangle$ and $\langle\mathcal{Q}\rangle=\langle\mathcal{P}\cup\mathcal{Q}\rangle$ hold, where each condition can be tested by Result 1.

Our findings do not generalize to *nonconnected compact groups* (iii), nor are they implied by the representation theory of compact groups. In particular, finite groups with trivial quadratic symmetries $[S,U_\nu\otimes U_\nu]=0$ only (known as group designs [69]) do not contradict our work.

VI. CONCLUSION

We have presented a complete symmetry approach to decide Hamiltonian simulability, i.e., whether given drift and control Hamiltonians can simulate a target (effective) Hamiltonian in finite dimensions. Quadratic symmetries lead to an understanding that allows one to algebraically prove simulability in classes of many-body systems where the usual computational assessment via the Lie closure is infeasible. This is exemplified by proving simulability for interesting cases of the central-spin model (see the Appendix) for which only very restricted cases were addressed before [63].

Achievability of specific target interactions is particularly important for fault tolerance, where the simulation of a particular Hamiltonian (or universality) is needed only on logical subspaces and not globally. While *linear* symmetries have often been used in those cases [70–73], going a step further by applying quadratic symmetries to ensure controllability or simulability on a noise-protected subspace could be an interesting application, simplifying complicated system-algebraic analysis. For instance, in Ref. [74], we examined standard scenarios of noise-protected subspaces, where controllability was (moderately) easy to assess. However, in more realistic settings, analyzing quadratic symmetries and their restrictions to protected subspaces is anticipated to be much easier than establishing Lie closures over restricted subspaces.

Moreover, our results on *quadratic* symmetries distinguishing local properties from global ones can be generalized into an overarching framework that encapsulates concurrence (Example 1) and links naturally to entanglement detection via a *quadratic* invariant of the quantum system under local transformations in [75–78].

Our findings imply that for *any* nonsimulable interaction, a related resource is lacking. In Example 1, it simply was entanglement, but more generally we can characterize lacking resources as induced by conserved quantities arising from quadratic symmetries. This paves the way toward a resource theory of quantum simulability.

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APPENDIX: CENTRAL-SPIN CONTROLLABILITY FOR DIFFERENT LEVELS OF GENERALITY

In this Appendix, we analyze under which conditions on the coupling coefficients J_k the central spin is controllable in Example 3. We collect proofs for this controllability under varying assumptions. Recall the set $\mathcal{P} = \{iH_1, iH_2\}$ of control interactions, where $iH_1 = iX_1 + i\sum_{k=2}^n J_k(X_1X_k+Y_1Y_k+Z_1Z_k)$ and $iH_2 = iZ_1$, as well as the target interaction $\mathcal{Q} = \{iX_1\}$. Assuming that condition (A) of Result 1 holds, there exists an element iC in the center of $\langle\mathcal{P}\cup\{iX_1\}\rangle$ such that $iX_1+iC \in \langle\mathcal{P}\rangle$. Since $iZ_1 \in \langle\mathcal{P}\rangle$, one obtains $-[iZ_1,[iZ_1,iX_1+iC]]/4 = iX_1 \in \langle\mathcal{P}\rangle$. Thus, it follows that it suffices to verify condition (A) in the different cases below, which is equivalent to showing that $D(iX_1)v = 0$ holds for all vectors $v \in \mathbb{C}^{d^4}$ with $d := 2^n$ and $D(iH_1)v = D(iH_2)v = 0$. Here, the linear operator

$$D(M) := [\mathbb{1}_{d^2}\otimes(M\otimes\mathbb{1}_d+\mathbb{1}_d\otimes M) \\ -(M\otimes\mathbb{1}_d+\mathbb{1}_d\otimes M)^t\otimes\mathbb{1}_{d^2}] \in \mathbb{C}^{d^4\times d^4}$$

is a shortcut in order to define the linear equations $D(M)v = 0$ for the matrix $M \in \mathbb{C}^{d\times d}$ and quadratic symmetries S where $v := \mathrm{vec}(S)$. One naturally obtains that both of the equations $[D(M_1),D(M_2)] = D([M_1,M_2])$ and $\exp[D(M_1)]D(M_2)\exp[-D(M_1)] = D[\exp(M_1)M_2\exp(-M_1)]$ hold for all matrices M_1, M_2.

Proposition 1. The interaction iX_1 can be simulated if all couplings J_k are either (a) equal, i.e., $J_k = J$, (b) equal up to an odd integer o_k, i.e., $J_k = Jo_k$ where o_k may depend on k, or (c) $\mathbb{Q}$-linear independent.

Proof. Let us consider the two definitions $i\tilde{H}_{\mathbf{zz}} := i\sum_{k=2}^n J_kZ_1Z_k = iH_1 + [iH_2,[iH_2,iH_1]]/4 \in \langle\mathcal{P}\rangle$ and $i\tilde{H} := iX_1 + i\sum_{k=2}^n J_k(X_1X_k+Y_1Y_k) = iH_1 - i\tilde{H}_{\mathbf{zz}} \in \langle\mathcal{P}\rangle$. We assume in the following that $D(iH_1)v = D(iH_2)v = D(i\tilde{H}_{\mathbf{zz}})v = D(i\tilde{H})v = 0$ holds in order to prove $D(iX_1)v = 0$.

The joint eigenbasis of the operators $D(iZ_k/2)$ and $D(iZ_1Z_k/2)$ for $k \in \{2,\ldots,n\}$ is given by the computational basis, and its basis vectors are $w(b) = |b_1\rangle\otimes\cdots\otimes|b_{4n}\rangle$ with $b_k \in \{0,1\}$, $|0\rangle := (0,1)^t$, and $|1\rangle := (1,0)^t$. This implies that the eigenvalue equations are $D(iZ_k/2)w(b) = i\mu_k(b)w(b)$ and $D(iZ_1Z_k/2)w(b) = i\lambda_k(b)w(b)$, and the corresponding eigenvalues are given by

$$\mu_k(b) = \tfrac{1}{2}(-s_k - s_{n+k} + s_{2n+k} + s_{3n+k}),$$

$$\lambda_k(b) = \tfrac{1}{2}(-s_1s_k - s_{n+1}s_{n+k} + s_{2n+1}s_{2n+k} + s_{3n+1}s_{3n+k}),$$

where $\mu_k(b) \in \{-2,-1,0,1,2\}$, $\lambda_k(b) \in \{-2,-1,0,1,2\}$, and $s_j := 2b_j - 1$. By checking all of the 2^8 cases for $s_{en+1}, s_{en+k} \in \{-1,+1\}$ and $e \in \{0,1,2,3\}$, one concludes that $\mu_k(b) \bmod 2 = \lambda_k(b) \bmod 2$ holds if $D(iZ_1)w(b) = 0$. Recall that $D(iZ_1)v = D(i\tilde{H}_{zz})v = 0$ and expand v as $v = \sum_b \alpha_b w(b)$. It follows that the equations $D(iZ_1)w(b) = 0$ and $D(i\tilde{H}_{zz})w(b) = 0$ hold for $\alpha_b \neq 0$ as each $w(b)$ is an eigenvector of $D(iZ_1)$ and $D(i\tilde{H}_{zz}) = \sum_{k=2}^n 2J_k\,D(iZ_1Z_k/2)$. Assuming $D(iZ_1)w(b) = 0$, this also means that the relation $\mu_z(b) \bmod 2 = \lambda_{zz}(b) \bmod 2$ holds for the eigenvalue $i\mu_z(b)$ of $\sum_{k=2}^n D(iZ_k/2)$ and the eigenvalue $i\lambda_{zz}(b)$ of $\sum_{k=2}^n D(iZ_1Z_k/2)$. Moreover, we obtain for $\alpha_b \neq 0$ that $0 = D(i\tilde{H}_{zz})w(b) = [i\sum_{k=2}^n 2J_k\lambda_k(b)]w(b)$ and, consequently, $\sum_{k=2}^n 2J_k\lambda_k(b) = 0$.

The proof depends now on the particular cases, and we prove in each case that $\mu_z(b) \bmod 2 = 0$: For case (a) with $J_k = J$, it follows that $\lambda_{zz}(b) = \sum_{k=2}^n \lambda_k(b) = 0$. This implies that $\mu_z(b) \bmod 2 = 0$. In case (b), we obtain $J_k = Jo_k$ and $\lambda_{zz}(b) \bmod 2 = \sum_{k=2}^n \lambda_k(b) \bmod 2 = \sum_{k=2}^n o_k\lambda_k(b) \bmod 2 = 0$, which also shows that $\mu_z(b) \bmod 2 = 0$. For case (c), $\sum_{k=2}^n 2J_k\lambda_k(b) = 0$ means that $\lambda_k(b) = 0$ for all k since the couplings J_k are $\mathbb{Q}$-linear independent and $\lambda_k(b) \in \mathbb{Z}$. In particular, it follows that $\lambda_{zz}(b) = \sum_{k=2}^n \lambda_k(b) = 0$, which proves again that $\mu_z(b) \bmod 2 = 0$.

Define the operator

$$W := \exp\left[\pi \sum_{k=2}^{n} D(iZ_k/2)\right].$$

Using the properties of $\sum_{k=2}^{n} D(iZ_k/2)$, one gets that the equation $Ww(b) = e^{i\mu_z(b)\pi}w(b) = w(b)$ holds for each $w(b)$ with $\alpha_b \neq 0$, where the last equality follows from $\mu_z(b) \bmod 2 = 0$. Thus, we obtain $Wv = W\sum_b \alpha_b w(b) = \sum_b \alpha_b W w(b) = \sum_b \alpha_b w(b) = v$. We also have that $WiD(X_1X_k+Y_1Y_k)W^\dagger = iD[G(X_1X_k+Y_1Y_k)G^\dagger]$, using the notation

$$G := \exp\left(\pi \sum_{k=2}^{n} iZ_k/2\right) = \prod_{k=2}^{n} \exp(\pi\, iZ_k/2) = \prod_{k=2}^{n} iZ_k.$$

It follows that $WiD(X_1X_k+Y_1Y_k)W^\dagger = iD[\prod_{k',k''=2}^{n} (iZ_{k'})(X_1X_k+Y_1Y_k)(-iZ_{k''})] = -iD(X_1X_k+Y_1Y_k)$ since $Z_kX_kZ_k = -X_k$ and $Z_kY_kZ_k = -Y_k$. Naturally, $WD(iX_1)W^\dagger = D(iX_1)$ is also satisfied.

One can now verify that

$$\begin{aligned} 0 &= WD(i\tilde{H})v = WD(i\tilde{H})W^\dagger W v \\ &= \left[D(iX_1) - \sum_{k=2}^{n} iJ_k D(X_1X_k+Y_1Y_k)\right]v \\ &= D(i\tilde{H})v - 2\sum_{k=2}^{n} iJ_k D(X_1X_k+Y_1Y_k)v. \end{aligned}$$

This implies $\sum_{k=2}^{n} iJ_k D(X_1X_k+Y_1Y_k)v = 0$, and one concludes that $D(i\tilde{H})v - \sum_{k=2}^{n} iJ_k D(X_1X_k+Y_1Y_k)v = D(iX_1)v = 0$. ■

The techniques in the proof of Proposition 1 can be generalized in order to establish the following result:

Proposition 2. The interaction iX_1 can be simulated if $J_k = J$ for $2 \leqslant k \leqslant n_0$ and $J_k = 2J$ for $n_0 < k \leqslant n$.

Proof. We establish again all the properties of the first two paragraphs in the proof of Proposition 1. Then, it follows that $\sum_{k=2}^{n_0} J\lambda_k(b) + \sum_{k=n_0+1}^{n} 2J\lambda_k(b) = 0$. Let $i\mu_z^{(0)}(b)$ be the eigenvalue of $\sum_{k=2}^{n_0} D(iZ_k/2)$. One obtains that $\mu_z^{(0)}(b) \bmod 2 = 0$ for each $w(b)$ with $\alpha_b \neq 0$. Define the operator

$$W^{(0)} := \exp\left[\pi \sum_{k=2}^{n_0} D(iZ_k/2)\right].$$

We apply the properties of $\sum_{k=2}^{n_0} D(iZ_k/2)$ and conclude that the equation $W^{(0)}w(b) = e^{i\mu_z^{(0)}(b)\pi}w(b) = w(b)$ holds for each element $w(b)$ satisfying $\alpha_b \neq 0$, where the last equality follows from $\mu_z^{(0)}(b) \bmod 2 = 0$. Thus, we obtain $W^{(0)}v = W^{(0)}\sum_b \alpha_b w(b) = \sum_b \alpha_b W^{(0)}w(b) = \sum_b \alpha_b w(b) = v$. We also have that $W^{(0)}iD(X_1X_k+Y_1Y_k)(W^{(0)})^\dagger = iD[G^{(0)}(X_1X_k+Y_1Y_k)(G^{(0)})^\dagger]$ using the notation

$$G^{(0)} := \exp\left(\pi \sum_{k=2}^{n_0} iZ_k/2\right) = \prod_{k=2}^{n_0} \exp(\pi\, iZ_k/2) = \prod_{k=2}^{n_0} iZ_k.$$

It follows that

$$\begin{aligned} &W^{(0)}iD(X_1X_k+Y_1Y_k)(W^{(0)})^\dagger \\ &\quad = iD\left[\prod_{k',k''=2}^{n_0} (iZ_{k'})(X_1X_k+Y_1Y_k)(-iZ_{k''})\right] \\ &\quad = -iD(X_1X_k+Y_1Y_k), \end{aligned}$$

if $2 \leqslant k \leqslant n_0$ since $Z_kX_kZ_k = -X_k$ and $Z_kY_kZ_k = -Y_k$, and $W^{(0)}iD(X_1X_k+Y_1Y_k)(W^{(0)})^\dagger = iD(X_1X_k+Y_1Y_k)$ if $k > n_0$. Naturally, $W^{(0)}D(iX_1)(W^{(0)})^\dagger = D(iX_1)$ is also satisfied.

One can now verify that

$$\begin{aligned} 0 &= W^{(0)}D(i\tilde{H})v = W^{(0)}D(i\tilde{H})(W^{(0)})^\dagger W^{(0)}v \\ &= \left[D(iX_1) - \sum_{k=2}^{n_0} iJD(X_1X_k+Y_1Y_k) \right.\\ &\qquad \left. + \sum_{k=n_0+1}^{n} 2iJD(X_1X_k+Y_1Y_k)\right]v \\ &= D(i\tilde{H})v - 2\sum_{k=2}^{n_0} iJD(X_1X_k+Y_1Y_k)v, \end{aligned}$$

which implies $\sum_{k=2}^{n_0} iJ_k D(X_1X_k+Y_1Y_k)v = 0$. Thus, one can conclude that $D(i\tilde{H})v - \sum_{k=2}^{n_0} iD(X_1X_k+Y_1Y_k)v = D(i\tilde{H}^{(1)})v = 0$, where we introduced the notation $i\tilde{H}^{(1)} := iX_1 + i\sum_{k=n_0+1}^{n} 2J(X_1X_k+Y_1Y_k)$.

Furthermore, the equation $D(i\tilde{H}_{zz})v = D(i\tilde{H}^{(1)})v = D(iH_2)v = 0$ implies the important commutator identity $[[[D(i\tilde{H}^{(1)}),D(iH_2)],D(i\tilde{H}^{(1)})],D(i\tilde{H}_{zz})]v = 0$. In addition, we have

$$\begin{aligned} &[[[D(i\tilde{H}^{(1)}),D(iH_2)],D(i\tilde{H}^{(1)})],D(i\tilde{H}_{zz})] \\ &\quad = D([[[\tilde{H}^{(1)},H_2],\tilde{H}^{(1)}],\tilde{H}_{zz}]) = 64J^2 D\left(i\sum_{k=n_0+1}^{n} Y_k\right). \end{aligned}$$

Thus, $D(i\sum_{k=n_0+1}^{n} Y_k)v = 0$. Now, we also get that

$$\begin{aligned} 0 &= \left[\left[D(i\tilde{H}_{zz}),D\left(i\sum_{k=n_0+1}^{n} Y_k\right)\right],D\left(i\sum_{k=n_0+1}^{n} Y_k\right)\right]v \\ &= -4D\big(i\tilde{H}_{zz}^{(1)}\big)v, \end{aligned}$$

where $i\tilde{H}_{zz}^{(1)} := i\sum_{k=n_0+1}^{n} 2JZ_1Z_k$. Considering the expansion $v = \sum_b \alpha_b w(b)$, we obtain from $D(i\tilde{H}_{zz}^{(1)})v = 0$ that the condition $\lambda_{zz}^{(1)}(b) = 0$ holds for the eigenvalue $i\lambda_{zz}^{(1)}(b)$ of $\sum_{k=n_0+1}^{n} D(iZ_1Z_k/2)$ with respect to a vector $w(b)$ with $\alpha_b \neq 0$. As we have for any $w(b)$ with $D(iZ_1)w(b) = 0$ that the eigenvalue $i\mu_z^{(1)}(b)$ of $\sum_{k=n_0+1}^{n} D(iZ_k/2)$ satisfies $\lambda_{zz}^{(1)}(b) \bmod 2 = \mu_z^{(1)}(b) \bmod 2$, thus we can conclude that $\mu_z^{(1)}(b) \bmod 2 = 0$ for b with $\alpha_b \neq 0$. We can now define the operator

$$W^{(1)} := \exp\left[\pi \sum_{k=n_0+1}^{n} D(iZ_k/2)\right].$$

Using the properties of $\sum_{k=n_0+1}^{n} D(iZ_k/2)$, one gets that the equation $W^{(1)}w(b) = e^{i\mu_z^{(1)}(b)\pi}w(b) = w(b)$ holds for each $w(b)$ with $\alpha_b \neq 0$, where the last equality follows from $\mu_z^{(1)}(b) \bmod 2 = 0$. Thus, we obtain $W^{(1)}v = W^{(1)}\sum_b \alpha_b w(b) = \sum_b \alpha_b W^{(1)}w(b) = \sum_b \alpha_b w(b) = v$. We also have that $W^{(1)} iD(X_1X_k{+}Y_1Y_k)(W^{(1)})^\dagger = iD[G^{(1)}(X_1X_k{+}Y_1Y_k)(G^{(1)})^\dagger]$ using the notation

$$G^{(1)} := \exp\left(\pi \sum_{k=n_0+1}^{n} iZ_k/2\right) = \prod_{k=n_0+1}^{n} \exp(\pi\, iZ_k/2)$$
$$= \prod_{k=n_0+1}^{n} iZ_k.$$

With these preparations, one can now verify that

$$0 = W^{(1)}D(i\tilde{H}^{(1)})v = W^{(1)}D(i\tilde{H})(W^{(1)})^\dagger W^{(1)}v$$
$$= \left[D(iX_1) - 2\sum_{k=n_0+1}^{n} iJ\,D(X_1X_k{+}Y_1Y_k)\right]v$$
$$= D(i\tilde{H})v - 4\sum_{k=n_0+1}^{n} iJ\,D(X_1X_k{+}Y_1Y_k)v,$$

which hence implies $\sum_{k=n_0+1}^{n} iJ_k D(X_1X_k{+}Y_1Y_k)v = 0$. Consequently, one can finally conclude that $D(i\tilde{H}^{(1)})v - \sum_{k=n_0+1}^{n} 2iJ\,D(X_1X_k{+}Y_1Y_k)v = D(iX_1)v = 0$. ■

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[44] The center of a set $\mathcal{M}$ of matrices contains all $M_1 \in \mathcal{M}$ that commute (i.e., $[M_1,M_2] = 0$) with every $M_2 \in \mathcal{M}$.

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[47] The interaction $iH\otimes\mathbb{1}_d+\mathbb{1}_d\otimes iH$ generates the unitary $\exp(-itH)\otimes\exp(-itH) = \exp[-t(iH\otimes\mathbb{1}_d+\mathbb{1}_d\otimes iH)]$.

[48] The $d^2\times d^2$ matrix $K_{d,d}$ [19, 49, 50] permutes $A,B \in \mathbb{C}^{d\times d}$ in $K_{d,d}(A\otimes B) = (B\otimes A)K_{d,d}$, which implies $K_{d,d} \in \mathcal{M}^{(2)}$ as $K_{d,d}(M\otimes\mathbb{1}_d+\mathbb{1}_d\otimes M) = (M\otimes\mathbb{1}_d+\mathbb{1}_d\otimes M)K_{d,d}$.

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