Nonperturbative \( k \)-body to two-body commuting conversion Hamiltonians and embedding problem instances into Ising spins

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An algebraic method has been developed which allows one to engineer several energy levels including the low-energy subspace of interacting spin systems. By introducing ancillary qubits, this approach allows \( k \)-body interactions to be captured exactly using two-body Hamiltonians. Our method works when all terms in the Hamiltonian share the same basis and has no dependence on perturbation theory or the associated large spectral gap. Our methods allow problem instance solutions to be embedded into the ground energy state of Ising spin systems. Adiabatic evolution might then be used to place a computational system into its ground state.

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This work considers an important problem. Given a Hamiltonian comprised solely of one-body and two-body terms, from this Hamiltonian, and with the aid of ancillary qubits, is it possible to construct the ground states of a Hamiltonian containing \( k \)-body terms with respect to a suitable subspace? In both the classical and quantum cases, this problem is particularly important when considering the physical complexity of interacting spin systems evolving into their lowest energy configuration [1–4] or the equivalent computational task of determining the ground state [5,6].

The ground state energy problem has long been considered in the realm of classical complexity theory with well-known results appearing in work such as [1,5]. The extension to quantum complexity classes was prompted when Kitaev [6], inspired by ideas from Feynman [7], showed that the ground state energy problem of the five-local (that is, five-body) random field quantum spin model was complete for the quantum analog of the class \( NP \). Thus it was shown that the five-local Hamiltonian was quantum-Merlin-Arthur-complete (QMA-complete) and the quest to determine the complexity of various spin models began [8–15].

Ideas from the theory of quantum computation have also led to the use of ground state properties of quantum systems for computation [3,16,17]. This is known as the adiabatic model of quantum computation [3,16]—in which a driving Hamiltonian is slowly replaced, most often with a commuting Hamiltonian with a ground state spin configuration representing a problem instance solution.

At the heart of the construction of the QMA-completeness proofs lies the development of methods to engineer low-energy effective Hamiltonians, which approximate \( k \)-body interactions, using at most two-body terms [10–12]. To date, all known methods require the introduction of a large spectral gap, where the magnitude of the gap improves only an approximate low-energy effective Hamiltonian. It would be desirable if one could (i) remove the spectral gap dependence by capturing the low-energy effective subspace exactly and (ii) develop a systematic method to engineer multiple energy subspaces, including any ground state.

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The present paper addresses both of these problems. Somewhat surprisingly, it is possible to remove dependence on the large spectral gap by allowing the state of the ancillary mediator qubits (facilitating the coupling) to follow the state of the qubits being coupled. In application, care is taken to ensure that the active role of the mediator qubits is appropriate for any given application. In many cases, this new approach allows ground states of \( k \)-body interactions to be captured exactly using two-body interactions; under the restriction that all terms in the Hamiltonian share the same basis.

Structure. The remainder of this paper begins with a short Introduction, followed by Sec. II, which explains how the ground states of three-body Hamiltonians can be used to embed any Boolean function (and for that matter, any switching circuit). Section III reduces the three-local Hamiltonians used in Sec. II to the case of two-local Hamiltonians: In addition, we prove Theorem III.1, which states the existence of an efficient method to construct Hamiltonians that simulate Boolean functions containing \( k \)-variable couplings (i.e., \( x_1 \land x_2 \land \cdots \land x_k \)). In Sec. IV we construct two-body Hamiltonians that exactly capture the ground space of \( k \)-body Hamiltonians of the form \( J \sigma_1 \otimes \sigma_2 \otimes \cdots \otimes \sigma_k \). Section IV also contains a proof of Theorem IV.1, which states the existence of a method to construct several energy subspaces of a given Hamiltonian—a necessity for certain applications.

In addition to the main body of the present paper, Appendix A presents a proof of a tailored variant of the projection Lemma [8,10,17]. This is followed by Appendix B which explains Karnaugh maps—key to an algebraic reduction method relied on during several derivations. We make use of standard quantum computing notation and background information [6,8] as well as that for discrete functions and circuits [18,19].

I. INTRODUCTION

Let us represent an Ising spin with index \( i \) by the variable \( s_i \in \{+1,-1\} \). One could also represent variable \( s_i \) in terms of binary variable \( x_i \in \{0,1\} \) as \( s_i = 1 - 2x_i \), which we will denote as \( |x_i\rangle \). A single spin system can be acted on by linear com-
bimations of operators taken from the set \{1, \pm \sigma\}, where the identity operator \(1\) can be scaled to ensure positivity-semidefiniteness and the operator \(\sigma\) has eigenvectors \([0]\) and \([1]\) with respective eigenvalues \(+1\) and \(-1\). The energy levels of the Hamiltonian operator \(\frac{1}{2}(1+\sigma_i)\left[\frac{1}{2}(1-\sigma_j)\right]\) corresponding to the states \([0]\) and \([1]\) are 1 and 0 [0 and 1]. Addition of the operator \(\frac{1}{2}(1+\sigma_i)\left[\frac{1}{2}(1-\sigma_j)\right]\) adds an energy penalty to the state \([0]\) \([1]\) and can be thought of as negation (assignment) of variable \(x_i\).

In the case of two Ising spins, a complete basis of configurations is \([00]\), \([01]\), \([10]\), and \([11]\). Let us add scaled sums of a coupling term to our Hamiltonian: \(\pm \sigma_i \sigma_j\). One can think of adding the operator \(\frac{1}{2}(1-\sigma_i \sigma_j)\) as a logical equality operation (i.e., the characteristic function \(x_i \Leftrightarrow x_j\) is true) and the operator \(\frac{1}{2}(1+\sigma_i \sigma_j)\) as a logical inequality operation (i.e., \(x_i \Leftrightarrow x_j\) is true) between spins. For example, assume we act on a dual spin system with the Hamiltonian for inequality: the ground state is in span\([01],[10]\), so any vector that corresponds to two spin variables being equal (e.g., span\([11],[00]\)=span\(\{i\}=∀x,y\in[0,1]\}) receives an energy penalty.

We have shown how to set single spin variables and how to apply equality and inequality operations between two spins. These operations, however, do not form a convenient logical system [20]. This will be done next, in Secs. II and III, by defining Hamiltonians with ground state spin configurations representing logical operations such as the AND (\(\wedge\)) gate, the OR (\(\vee\)) gate, etc. We know that these dual arithmetic operations require at least three spins as \(x_i \wedge x_j = z_s\). What we need is to find a way to set the low-energy subspace of three spins \(s_i, s_j,\) and \(z_s\) to be, for instance, the logical AND of the spins \(s_i \wedge s_j = z_s\). This assignment turns out to be possible working in the energy basis of a Hamiltonian equipped with a commuting local field and coupling term, such as an Ising Hamiltonian [21]:

\[
H_{\text{Ising}} = \sum_i h_i \sigma_i + \sum_{i,j} J_{ij} \sigma_i \sigma_j.
\]


II. GROUND STATE SPIN LOGIC

Consider some Hamiltonian \(H\) acting on a Hilbert space \(\mathcal{H}\) that is a sum of the vectors spanned by the subspace \(\mathcal{L}\) and the orthogonal component of \(\mathcal{L}\) written as \(\mathcal{L}^\perp\), thus \(\mathcal{H}=\mathcal{L}^\perp + \mathcal{L}\). The lowest eigenvalue of \(H\) will be denoted as \(\lambda(H)\).

Now let \(\Pi_{\mathcal{L}} \equiv (1 - \mathcal{L}^\perp)\) be defined as a projector onto \(\mathcal{L}\). Then \(\Pi_{\mathcal{L}}H_{\mathcal{L}}\Pi_{\mathcal{L}}\) is the restriction of \(H\) to the subspace \(\mathcal{L}\)—let us write this restriction as \(\mathcal{H}_{\mathcal{L}}\).

To develop the logic, consider the Hamiltonian \(\mathcal{H}_{\mathcal{prop}}\) such that \(\mathcal{H}_{\mathcal{prop}}|\mathcal{L}\rangle = 0\) and \(\mathcal{H}_{\mathcal{prop}}|\mathcal{L}^\perp\rangle \equiv \delta|\mathcal{H}_{\mathcal{in}}\rangle\) where \(\mathcal{H}_{\mathcal{in}}\) is a perturbation later used to set the circuits inputs, the norm \(\|\|\) is the magnitude of the Hamiltonians largest eigenvalue, and \(\delta\) is the spectral gap between the \(\mathcal{L}^\perp\) and \(\mathcal{L}\) subspaces. We are faced with the task of ensuring that \(\mathcal{H}_{\mathcal{prop}}|\mathcal{L}\rangle = 0\) is a zero eigenspace when \(\mathcal{L}\) spans the truth table of the logical operation of interest (e.g., \(\mathcal{L} = \text{span}\{[1],[01],[10],[11]\}\) for the logical AND, \(\mathcal{L} = \text{span}\{[1],[01],[0],[11]\}\) for the logical OR, \(\mathcal{L} = \text{span}\{[1],[01],[10],[11]\}\) for the logical NOT). Let \(\mathcal{L}\) be the low-energy subspace representing the truth table in the binary operations. Explicitly, in the case of logical AND, \(\mathcal{L} = \text{span}\{[1],[01],[10],[11]\}\) \(\mathcal{L} = \text{span}\{[0],[01],[0],[11]\}\) \(\mathcal{L} = \text{span}\{[1],[01],[10],[11]\}\) for the logical NOT, \(\mathcal{L} = \text{span}\{[1],[01],[10],[11]\}\) for the logical OR.

One can add a perturbation, \(\mathcal{H}_{\mathcal{in}}\), to set the circuits inputs. We will write this as a projector onto the \(n\) long binary bit vector \(x\). This one-local projector has the form

\[
\Pi_k = |x\rangle\langle x| = \prod_{i=1}^{n} \left[ 1 + (-1)^{1-s_i} \sigma_i \right].
\]

Now upper bound \(\|\mathcal{H}_{\mathcal{in}}\|\) (for all two input and single output gates [26]) as \(\|\mathcal{H}\|\) \(\leq\). This implies that the spectral gap \(\delta\) is greater than 2. By noticing that \(\forall j,k\),

\[
\langle s_j | H | s_k \rangle^* = \lambda | s_j \rangle \langle s_k |
\]

and

\[
\langle s_j | H | s_k \rangle + \langle s_k | H | s_j \rangle = 0,
\]

where \(\langle s_j | \in \mathcal{L}\) and \(\langle s_k | \in \mathcal{L}^\perp\), one recovers the strict equality, \(\lambda(H)_{\mathcal{L}}\) and \(\lambda(H)_{\mathcal{L}^\perp}\) (see Lemma II.2).

Using combinations of these ground state logic gates, we will perform computations. For example, write the Hamiltonian with a low-energy subspace in

\[
\text{span}\{[1],[01],[10],[11]\}\]

as \(H_{\mathcal{L}}(x_1,x_2,x_3)\) and, with \(y_3\) defined in Eq. (2), write the Hamiltonian with a low-energy subspace in

\[
\text{span}\{[0],[01],[0],[11]\}\]

as \(H_{\mathcal{L}}(x_1,x_2,y_3)\). Then the proposition \(x_1 \wedge x_2 \vee x_3 = z_s\) is constructed as a sum of terms:

\[
H_{\mathcal{prop}} = H_{\mathcal{L}}(x_1,x_2,y_3) + H_{\mathcal{L}}(x_3,y_3,z_s) + H_{\mathcal{in}}
\]

and the circuits input, \(H_{\mathcal{in}}\), is yet to be defined (see Fig. 1).

FIG. 1. Illustrating the mapping between circuits (with Boolean variables \(x_i\) and spins \(z_s\)) for the example given in Eq. (3). One can use any number of methods to embed logical networks [18] into the ground space of Hamiltonians.
where each gate is defined by its type taken from an input variables and consists of a finite number of gates, local Hamiltonians. Before continuing to our two-local reduction we see the freely available standard reference additional background information on Boolean functions and an asynchronous low-energy subspace would be spanned by all vectors where

\[
\text{O} = 101 \text{ and } 110 \text{, which acts on the circuits output } z, \text{ then the low-energy subspace would be spanned by all vectors where the output } z \text{ is } 1 \text{ [27]. As seen from Table II, this subspace is in }
\]

\[
\\text{span}\{001\}|1\rangle|0\rangle, |011\}|1\rangle|0\rangle, |101\}|1\rangle|0\rangle, |110\}|1\rangle|1\rangle, |111\}|1\rangle|1\rangle, \]

where we adhere to the ordering \[|x_1x_2x_3\rangle|z\rangle|y\rangle\]. If instead we were to add the perturbation \(H_{\alpha}\) to the qubit labeled \(|y\rangle\), the ground space would be spanned by \{|110\}|1\rangle|1\rangle, |111\}|1\rangle|1\rangle\}.

To complete our reduction, the three-local Hamiltonians, just described, will be reduced in the next section to two-local Hamiltonians. Before continuing to our two-local reduction, let us state Lemma II.2 and Theorem II.1—the proof of which is implied by the results of this section. Here we choose a finite set \(\Omega\) of one-output Boolean functions as the basis. Then, an \(\Omega\)-circuit works for a fixed number of Boolean input variables and consists of a finite number of gates, where each gate is defined by its type taken from \(\Omega\). (For additional background information on Boolean functions and switching circuits see the freely available standard reference [18].)

**Theorem II.1.** Let \(f\) be a switching function given as the map \(f:\{0,1\}^k \rightarrow \{0,1\}^m\) for finite \(k\) and \(m\). Now let there be an asynchronous \(\Omega\)-circuit computing \(f\). Then there exists an \(\Omega\)-circuit embedding into the ground space of a three-local Hamiltonian, \(H_3\), such that (i) the norm of the Hamiltonian \(\|H_3\|\) is constant and, in particular, independent of the size of \(f\), the \(\Omega\)-circuit, as well as \(k\) and \(m\). (ii) The \(\Omega\)-circuit embedding is upper bounded by a number of qubits \(O(1)\)—reducible to the number of classical gates required on the same lattice.

**TABLE I.** Left column: possible assignments of the variables \(x_1\), \(x_2\), and \(z\). Center column: illustrates the variable assignments that must receive an energy penalty \(\geq \delta\). Right column: truth table for \(H_\alpha(x_1, x_2, z) = 3z + x_1 \wedge x_2 - 2z \wedge x_1 - 2z \wedge x_2\), which has a null space \(L \in \text{span}\{x_1x_2\}|z\rangle|z\rangle = x_1 \wedge x_2 \forall x_1, x_2 \in \{0, 1\}\}.

<table>
<thead>
<tr>
<th>(x_1)</th>
<th>(x_2)</th>
<th>(z)</th>
<th>(z = x_1 \wedge x_2)</th>
<th>(H_\alpha(x_1, x_2, z))</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>0</td>
<td>0</td>
<td>1</td>
<td>001</td>
<td>(H_\alpha(001) = 3\delta)</td>
</tr>
<tr>
<td>0</td>
<td>1</td>
<td>0</td>
<td>010</td>
<td>(H_\alpha(010) = 0)</td>
</tr>
<tr>
<td>0</td>
<td>1</td>
<td>1</td>
<td>011</td>
<td>(H_\alpha(011) = \delta)</td>
</tr>
<tr>
<td>1</td>
<td>0</td>
<td>0</td>
<td>100</td>
<td>(H_\alpha(100) = 0)</td>
</tr>
<tr>
<td>1</td>
<td>0</td>
<td>1</td>
<td>101</td>
<td>(H_\alpha(101) = \delta)</td>
</tr>
<tr>
<td>1</td>
<td>1</td>
<td>1</td>
<td>111</td>
<td>(H_\alpha(111) = 0)</td>
</tr>
</tbody>
</table>

**TABLE II.** Ground state truth table generated for the Hamiltonian (3). The function output, \(z\), is equal to \(x_1 \wedge x_2 \lor x_3\). It is instructive to think of the variable \(x_3\) as a coupler that follows the variables \(x_1\) and \(x_2\) as \(y = x_1 \wedge x_2\).

<table>
<thead>
<tr>
<th>(x_1x_2x_3)</th>
<th>(z)</th>
<th>(y)</th>
</tr>
</thead>
<tbody>
<tr>
<td>000</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>001</td>
<td>1</td>
<td>0</td>
</tr>
<tr>
<td>010</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>011</td>
<td>1</td>
<td>0</td>
</tr>
<tr>
<td>100</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>101</td>
<td>1</td>
<td>0</td>
</tr>
<tr>
<td>110</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>111</td>
<td>1</td>
<td>1</td>
</tr>
</tbody>
</table>

An important technical tool used in our construction is a variant of the projection Lemma [8,10,17]—proven in Appendix A. Let us denote \(\mathcal{H}\) as a Hilbert space of interest and let \(H_1\) be some Hamiltonian. Consider a subspace \(\mathcal{L} \subset \mathcal{H}\) such that a Hamiltonian \(H_2\) has the property that \(\mathcal{L}\) is a 0 eigenspace and \(\mathcal{L}^\perp\) is an eigenspace of at least \(\delta > 2||H_1||\). Consider the Hamiltonian \(H = H_1 + H_2\), the projection lemma says that the lowest eigenvalue of \(H\), \(\lambda(H)\), is the lowest eigenvalue of \(H_1\) restricted to the subspace \(\mathcal{L}\)—that is \(\lambda(H_{|\mathcal{L}})\). Thus by adding \(H_2\) one adds a penalty (proportional to \(\delta\)) to any vector in \(\mathcal{L}^\perp\). To state the projection lemma (strict equality) we state the following.

**Lemma II.2.** Let \(H = H_1 + H_2\) be the sum of two Hamiltonians operating on some Hilbert space \(\mathcal{H} = \mathcal{L} + \mathcal{L}^\perp\). Denote \(\mathcal{L} = \text{span}\{|s\rangle \forall j\}\) and \(\mathcal{L}^\perp = \text{span}\{|s^\perp\rangle \forall k\}\) for finite \(j, k\). Consider the restriction \(H_{|\mathcal{L}} = 0\) and \(H_{|\mathcal{L}} \geq \delta > 2||H_1||\). Then, if \(\forall j, k, s_1, s_2 \in \mathcal{F}\) \(H_{|\mathcal{L}} s_1 = \lambda(s_1) s_1\) \(\forall k, H_{|\mathcal{L}} s_2 = \lambda(s_2) s_2\), \(s_1 H_{|\mathcal{L}} s_2\) + \(s_2 H_{|\mathcal{L}} s_1\) = 0 the following equality holds: \(\lambda(H) = \lambda(H_{|\mathcal{L}})\).

**III. TWO-LOCAL REDUCTION**

The main result of this section can be found in Table III. To develop this table we used the algebra of multilinear forms [19] and the Karnaugh map method from discrete mathematics [28]—which we review in Appendix B.

We consider multilinear forms that are maps \(f\) from the Boolean numbers to the reals, where the inputs and outputs are of finite size. For instance, the multilinear form for \text{AND} (or \text{OR}) is simply \(f_{\text{AND}} = x_1 \wedge x_2\) \(f_{\text{OR}} = x_1 + x_2 - 2x_1 \wedge x_2\). Hence one can express the Boolean equation \(f = x_1 \wedge x_2 \lor x_3\) with the polynomial \(f = x_1 \wedge x_2 + x_3 - x_1 \wedge x_2 \wedge x_3\). Let us first write the vector of integers:

\[
e^T = (c_0, c_1, c_2, c_3, c_4, c_5, c_6, c_7),
\]

representing the outputs of a multilinear function \(f\) over the three Boolean input arguments \(x_1\), \(x_2\), and \(x_3\). We wish to construct a canonical representation for any multilinear function of three variables in terms of the vector \(e\) from Eq. (4).

We will represent the negation of the variable \(x\) as \(\bar{x}\) (or using the notational equivalent \(\neg x\)) and canonically expand Eq. (4) as a sum of products:
TABLE III. Logical gadgets (Sec. III): The span of the zero energy ground space (L) of these gadget Hamiltonians represent the truth table of a given switching function in the spin variables (as, for instance, the AND function: \( L = \text{span}\{ |x_1x_2|z_\ast\}|z_\ast = x_1 \land x_2, \forall x_1, x_2 \in \{0, 1\}\}). This table includes all \( 16 = 2^5 \) possible Boolean functions with \( n = 2 \) inputs.

| Function | Two-local Hamiltonian \( H(x_1, x_2, z_\ast) = \frac{1}{2} (1 - \sigma_1) \) | Ground state (ordered: \( |x_1| |x_2| |z_\ast\) ) |
|-----------|---------------------------------------------------|----------------------------------|
| 0 = \( z_\ast \) | \( \frac{1}{2} (1 - \sigma_1) \) | \( \text{span}\{ |010|, |011|, |001|, |101|\} \) |
| 1 = \( z_\ast \) | \( \frac{1}{2} (1 + \sigma_1) \) | \( \text{span}\{ |010|, |011|, |001|, |101|\} \) |
| \( \bar{x}_1 \land \bar{x}_2 = \bar{z}_\ast \) | \( \frac{1}{2} (3 + \sigma_1 + \sigma_2 - 2 \sigma_1 \sigma_2 + \sigma_1 \sigma_2 - 2 \sigma_1 \sigma_2) \) | \( \text{span}\{ |001|, |010|, |100|, |110|\} \) |
| \( x_1 \land x_2 = \bar{z}_\ast \) | \( \frac{1}{2} (3 - \sigma_1 - \sigma_2 + 2 \sigma_1 \sigma_2 - 2 \sigma_1 \sigma_2 - 2 \sigma_1 \sigma_2) \) | \( \text{span}\{ |000|, |011|, |100|, |111|\} \) |
| \( x_1 \land \bar{x}_2 = \bar{z}_\ast \) | \( \frac{1}{2} (3 - \sigma_1 + \sigma_2 - 2 \sigma_1 \sigma_2 + \sigma_1 \sigma_2 - 2 \sigma_1 \sigma_2) \) | \( \text{span}\{ |000|, |010|, |101|, |111|\} \) |
| \( x_1 \lor x_2 = \bar{z}_\ast \) | \( \frac{1}{2} (4 + \sigma_1 + \sigma_2 - 2 \sigma_1 \sigma_2 + 2 \sigma_1 \sigma_2 - 3 \sigma_1 \sigma_2 - 3 \sigma_1 \sigma_2 - 3 \sigma_1 \sigma_2) \) | \( \text{span}\{ |000|, |001|, |100|, |101|\} \) |
| \( x_1 \lor \bar{x}_2 = \bar{z}_\ast \) | \( \frac{1}{2} (4 - \sigma_1 - \sigma_2 + 2 \sigma_1 \sigma_2 + 2 \sigma_1 \sigma_2 - 3 \sigma_1 \sigma_2 - 3 \sigma_1 \sigma_2) \) | \( \text{span}\{ |001|, |101|, |111|, |110|\} \) |
| \( x_1 \oplus x_2 = z_\ast \) | \( \frac{1}{2} (1 + \sigma_1 \sigma_3) \) | \( \text{span}\{ |000|, |100|, |101|, |011|\} \) |
| \( x_2 \oplus z_\ast \) | \( \frac{1}{2} (1 - \sigma_1 \sigma_3) \) | \( \text{span}\{ |000|, |100|, |101|, |011|\} \) |
| \( x_2 \oplus z_\ast \) | \( \frac{1}{2} (1 + \sigma_1 \sigma_3) \) | \( \text{span}\{ |000|, |100|, |101|, |011|\} \) |
| \( x_2 \oplus z_\ast \) | \( \frac{1}{2} (1 + \sigma_1 \sigma_3) \) | \( \text{span}\{ |000|, |100|, |101|, |011|\} \) |
| \( x_1 \lor x_2 = z_\ast \) | \( 4 + \sigma_1 \sigma_2 + (\sigma_1 + \sigma_2) \sigma_2 + 2 (1 - \sigma_1 - \sigma_2 - \sigma_1 \sigma_2) \sigma_1 - \sigma_2 \) | \( \text{span}\{ |000|, |011|, |101|, |111|\} \) |
| \( x_1 \lor x_2 = z_\ast \) | \( 4 - \sigma_1 \sigma_2 + (\sigma_1 + \sigma_2) \sigma_2 + 2 (1 - \sigma_1 - \sigma_2 - \sigma_1 \sigma_2) \sigma_1 - \sigma_2 \) | \( \text{span}\{ |010|, |001|, |111|, |100|\} \) |

\[
f(x_1, x_2, x_3) = c_0 \bar{x}_1 \bar{x}_2 x_3 + c_1 \bar{x}_1 \bar{x}_2 x_3 + c_2 \bar{x}_1 \bar{x}_2 x_3 + c_3 \bar{x}_1 \bar{x}_2 x_3 + c_4 \bar{x}_1 \bar{x}_2 x_3 + c_5 \bar{x}_1 \bar{x}_2 x_3 + c_6 \bar{x}_1 \bar{x}_2 x_3 + c_7 \bar{x}_1 \bar{x}_2 x_3.
\]

\[
(5)
\]

This expansion (5) forms a basis for the space of three-variable Hamiltonians, but to realize any of the eight terms requires three-body couplings. This motivates us to write a second canonical expansion, found from a change of variables in Eq. (5) and by expanding each term into its positive polarity form:

\[
f(x_1, x_2, x_3) = a_0 + a_1 x_1 + a_2 x_2 + a_3 x_3 + a_4 x_1 x_2 + a_5 x_1 x_3 + a_6 x_2 x_3 + a_7 x_1 x_2 x_3.
\]

\[
(6)
\]

This Eq. (6) also forms a basis for the space of realizable Hamiltonians of three-spins. In this suggestive form, however, we can truncate Eq. (6) past second order and consider the subclass of Hamiltonians that can be realized by setting \( a_7 = 0 \).

Out of the 16 possible functions of two-input and one-output variable, it can be proven that only two are not realizable using three-spins. These are the two-local penalty Hamiltonians for XOR (\( \oplus \)) and EQV (\( \odot \)) [29], which are each possible to realize by adding a single mediator qubit (as seen in Table III).

We will explain in detail how the positive-semidefinite AND penalty Hamiltonian, \( H_\land \), is derived. We anticipate that the details of our approach will aid others faced with Hamiltonian constructions. Let \( L \) be the null space of \( H_\land \) and let all higher eigenspaces be given as \( L^\perp \). The penalty Hamiltonian has a null space, \( L \), spanned by the vectors \( \{ |x_1x_2|z_\ast\} |z_\ast = x_1 \land x_2, \forall x_1, x_2 \in \{0, 1\}\}. Denote \( \delta \) as an energy penalty applied to any vector component in \( L^\perp \). Our goal is to develop a Hamiltonian that adds a penalty of at least \( \delta \) to any vector that does not satisfy the truth table of the AND gate—that is, we want to add an energy penalty to any vector with a component that lies in \( L^\perp \).

In order to make the penalty quadratic, one first constructs the Karnaugh map illustrated in Fig. 2(c) for the case \( x_1 \land x_2 = z_\ast \). This is done by examining Table I. In the rightmost column, all possible assignments for the variables \( x_1, x_2, \) and \( z_\ast \) are shown. The Karnaugh map is constructed by examining the second column. Whenever the variable \( z_\ast \) is not equal to the AND of the variables \( x_1 \) and \( x_2 \), a penalty of at least \( \delta \) must be applied, which ensures that vectors in the ground space satisfy \( |x_1| |x_2| |x_1 \land x_2| \). Any vector that must receive an energy penalty of \( \delta \) is depicted in the Karnaugh map with a dot (\( \ast \)).

Begin by noticing that any vector associated with cube number 4 must receive an energy penalty, so the 1-local field corresponding to the qubit with label \( z_\ast \) must be at least \( \delta \)—adding the term \( p_1z_\ast \) to the Hamiltonian, with the constraint \( p_1 \geq \delta \). Cube 3 must also receive an energy penalty of at least \( \delta \), adding the term \( p_2x_1 \land x_2 \) to the Hamiltonian \( H_\land \). With both penalties applied, vectors corresponding to cube 7 must be brought back to the null space—accomplished by subtracting the quadratic energy rewards \( r_1z_\ast \land x_1 \) and
We now have the necessary machinery in place to state two theorems that often needs to couple three Boolean variables. Let $f_k$ be a $k$-local multilinear form and let there be a Hamiltonian $H_k$ acting on the Hilbert space $\mathcal{H}_k$ such that $f_k = H_k$. Then there exists a two-local multilinear form, $f_2$, and corresponding Hamiltonian, $H_2$, acting on the Hilbert space $\mathcal{H}_2$ (where $\mathcal{H}_2 \subseteq \mathcal{H}_k$), with the same low-energy subspace of $H_2$ in span $\{|x\rangle \mid y = f_k(x), \forall x \in \{0,1\}^n, \forall y \in \{0,1\}^m \subseteq \mathcal{H}\}$. The number of mediator qubits required to realize $H_2$ is upper bounded by $O(\text{size}(f_3))$. In addition, the spectral gap of $H_2$ is bounded by the spectral gap of $H_k$.

Proof. To construct such a Hamiltonian, we will employ an inductive argument and consider a single (out of $w$) $k$-local term, $h_k = x_1 \land x_2 \land \cdots \land x_k$, that couples $k \geq 3$ Boolean variables. We will now show the existence of a two-local reduction requiring $(k-2)$ mediator qubits to embed $h_k$ into the ground state of a two-local Hamiltonian. Consider the two-local coupling $z \land x_1$ and add the Hamiltonian that forces an energy penalty whenever $z$ is not the Boolean AND of the variables $x_1$ and $x_2$. The two-local Hamiltonian is written as

$$H_2(x_1, x_2, z) = 1/2(-\sigma_1 \land -\sigma_2 + 2\sigma_1 \land -\sigma_2 + 2\sigma_1 \land \sigma_2 - 2\sigma_1 \land 2\sigma_1 \land \sigma_2),$$

where $H_2$ is found in Table III, and $z$ is a temporary variable. In words, the variable $z$ is coupled to $x_3$ and the penalty, $H_2$, forces $z$ to be equal to the Boolean product of $x_1$ and $x_2$—thereby creating the desired coupling with respect to the subspace spanned by $|x_1 x_2 x_3\rangle$, $\forall i \in \{1,2,3\}, x_i \in \{0,1\}$. For a $k$-local term $x_1 \land x_2 \land \cdots \land x_k$, this procedure is recursively repeated $k-2$ times. The reduction requires $w-(k-2)$ qubits to capture the low-lying eigenspace of $H_2$ with $H_3$.

Theorem III.2. Let $f$ be a switching function with a fixed number of inputs $k$ and outputs $m$. Let there be an asynchronous $\Omega$-circuit computing $f$ over the basis $\{\land, \lor, \lnot\}$. There exists an $\Omega$-circuit embedding into the ground state of a two-local Hamiltonian, $H_3$, such that (i) the norm of the Hamiltonian $\|H_3\|$ is constant and, in particular, independent of the size of $f$, the $\Omega$-circuit, $k$ as well as $m$. (ii) The $\Omega$-circuit embedding is upper bounded by a number of qubits $O(k)$-reducible to the number of classical gates required on the same lattice.

IV. THREE-LOCAL GADGET

We are concerned with constructing the ground state of the operator $J_3 \land \sigma_1 \land \sigma_2 \land \sigma_3$—which is a different task than coupling (that is, the AND product) three Boolean variables $x_1 \land x_2 \land x_3$. Without loss of generality, let us consider construction of the target Hamiltonian

$$H_{\text{target}} = Y + J_3 \land \sigma_1 \land \sigma_2 \land \sigma_3,$$

where $Y$ is diagonal in the $\sigma$ basis. We will write the spectrum of $\sigma_1 \land \sigma_2 \land \sigma_3$, in canonical (Boolean counting) order, as $\{1, -1, 1, -1, 1, -1\}$ [30]. Now the low-energy, $\lambda(\sigma_1 \land \sigma_2 \land \sigma_3) = -1$, eigenspace is given as...
\[ L = \text{span}([001], [010], [100], [111]) \]
and the high-energy, +1, eigenspace as
\[ L^\perp = \text{span}([000], [011], [101], [110]). \]

Over the complex field, the tensor product (\( \otimes \)) of two elements is simply their complex multiplicative (\( \cdot \)) product. With respect to the canonical order, the spin variables for this operator (11) form the product \( z_\ast = z_1 \cdot z_2 \cdot z_3 \), where \( \forall i, j \in \{+1, -1\} \), and so we consider the group homomorphism \( \{-1, +1, 1\} \rightarrow \{0, 1, 0\} \), where \( \oplus \) denotes modulo 2 sum (XOR);
\[
z_\ast = x_1 \oplus x_2 \oplus x_3, \ \forall x_1, x_2, x_3 \in \{0, 1\}^3.
\]

In what follows, we will present a general framework to construct the ground state of any operator in the \( \sigma \) basis and apply this approach to produce a three-local gadget requiring three mediator qubits. We will then focus our attention on optimization of this new three-local gadget, which is shown to be possible to realize using only two mediator qubits.

Let us state an overview of our approach. To capture both the low- and high-energy spectrum, while preserving the spectral gap, one will first write down a penalty Hamiltonian for the three-variable function \( \text{spectral gap} \), one will first write down a penalty Hamiltonian the low- and high-energy spectrum, while preserving the possibility to realize using only two mediator qubits. We will then apply this approach to produce a three-local gadget requiring three mediator qubits. We will then focus our attention on optimization of this new three-local gadget, which is shown to be possible to realize using only two mediator qubits.

\[ H = \frac{\delta}{2} [4 + \sigma_2 \sigma_3 + (\sigma_2 + \sigma_3) \sigma_4 + 2(1 - \sigma_2 - \sigma_3 - \sigma_4) \sigma_5 - \sigma_2 - \sigma_3 - \sigma_4] + \langle \sigma_1 \sigma_2 \rangle \tau_{x_4} \]

The ground space of the Hamiltonian (12) is given as
\[ L = \text{span}([001][00], [010][11], [100][11], [111][01]) \]
and the first excited space as
\[ L^\perp = \text{span}([000][01], [100][00], [110][00], [111][10]), \]
where the qubits are in ascending order: qubit 4 represents the Boolean EQV of qubits 2 and 3, while qubit 5 is the mediator qubit needed to construct the EQV function.

We will now state then prove Theorem IV.1 which allows one to construct not only the ground state, but several levels of the low-lying energy subspace of \( k \)-body interactions using only two-body Hamiltonians.

**Theorem IV.1.** Let \( H_k \) be a \( k \)-local Hamiltonian diagonal in any basis \( \sigma \) and let this Hamiltonian act on the Hilbert space \( \mathcal{H}_k \). Assert that \( H_k \) has a bounded norm, and let the strictly increasing list \( \{E_1, E_2, \ldots, E_k\} \) denote the eigenenergies of \( H_k \) formed by combing degeneracies, and label the corresponding eigenspaces as \( \{L_1, L_2, \ldots, L_k\} \), respectively. Then there exists a two-local Hamiltonian, \( H_2 \), with a low-lying spectrum isomorphic to that of \( H_k \). Moreover, \( H_2 \) is equivalent to \( H_k \) with respect to a subspace spanned by \( \{L_1, L_2, \ldots, L_k\} \). In particular, there exists a two-local reduction capturing the \( k \) energy subspaces \( \{L_1, L_2, \ldots, L_k\} \) in the low-energy subspace \( H_2 \).

**Proof.** Let us review the general method to construct ground states. First, determine \( L \), the low-energy subspace, and let \( E_k \) denote the ground state energy. One will next write a function, \( z_\ast = f(x_1, x_2, \ldots, x_n) \), that outputs 0 for all input vectors in \( L \), and for all other vectors the function will output 1. The ground state will be realized with respect to a subspace spanned by the qubits labeled \( [x_1], [x_2], \ldots, [x_n] \). To capture the desired ground space, a perturbation \( V = E_k[0][0] \) is added, which only acts on the qubit \( z_\ast \). Assume that we are instead interested in capturing several energy subspaces, with energies \( \{E_1, E_2, \ldots, E_k\} \), and let us label these spaces as \( \{L_1, L_2, \ldots, L_k\} \), respectively. We will construct a function with \( k \) outputs and repeat the process outlined above—this time acting on each respective \( j \)th function with the perturbation \( V = \sum_{j=1}^{k} E_j[0][0] \).

**V. CONCLUSION**

In this study, we have adapted a range of classical algebraic reduction methods to the construction of the low-lying energy subspace of \( k \)-local Hamiltonians using two-local Hamiltonians. Our methods do not rely on perturbation theory or the associated large spectral gap. We have examined explicit constructions of various useful \( k \)-local to two-local conversion Hamiltonians—including both those needed to embed logical functions as well as couple spin variables. We have found constructions of these Hamiltonians which are optimal in the number of introduced ancillary qubits. For
TABLE IV. Three-local gadgets. Top (Sec. III): Hamiltonian with a low-energy subspace that couples three Boolean variables. The state of the mediator qubit $\sigma_2$ is a function (the AND) of qubits 1 and 2. Bottom (Sec. IV): Hamiltonian with low-energy subspace that couples three spin variables for $\delta^2 > 2|\beta|$. The ground space, $\mathcal{L} = \text{span}([001],[010],[110])$, and the first excited space, $\mathcal{L}^+ = \text{span}([000],[110],[000], [110])$—the qubits are in ascending order: qubit 4 represents the Boolean EQV of qubits 2 and 3, while qubit 5 is the mediator qubit needed to construct the EQV function.

<table>
<thead>
<tr>
<th>Three-local coupling</th>
<th>Two-local Hamiltonian</th>
</tr>
</thead>
<tbody>
<tr>
<td>$J_{x_1 \wedge x_2 \wedge x_3}$</td>
<td>$\frac{1}{2}(4 - \sigma_1 - \sigma_2 + 3\sigma_1 + \sigma_1\sigma_2 - 2\sigma_1\sigma_2 + J_{x_1\sigma_2})$</td>
</tr>
<tr>
<td>$J_{\sigma_1 \otimes \sigma_2 \otimes \sigma_3}$</td>
<td>$\frac{1}{2}(4 + \sigma_2\sigma_3 + (\sigma_2 + \sigma_3)\sigma_1 + 2(1 - \sigma_1\sigma_3 - \sigma_3\sigma_2)\sigma_3 - \sigma_3 - \sigma_2 + J_{\sigma_1\sigma_2})$</td>
</tr>
</tbody>
</table>

Ease of reference, our results are summarized in Tables III and IV. In Theorem IV.1 we presented a method to construct several levels, including the ground state, of the low-lying energy subspace of $k$-body interactions using two-body Hamiltonians. Our methods have several applications in adiabatic quantum algorithm design and quantum complexity theory.

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APPENDIX A: PROJECTION LEMMA

We will now prove Lemma II 2 which is discussed in Sec. II. Consider first the case that $\lambda(H) \geq \lambda(H|_{\mathcal{L}})$. Denote by $|\eta\rangle \in \mathcal{L}$ the minimizing eigenvector of $H|_{\mathcal{L}}$ with eigenvalue $\lambda(H|_{\mathcal{L}})$. Since $H_2|\eta\rangle = 0$,

$$\langle \eta | H | \eta \rangle = \langle \eta | H_1 | \eta \rangle + \langle \eta | H_2 | \eta \rangle = \lambda(H|_{\mathcal{L}}).$$

Now consider actually minimizing over all vectors $|\zeta\rangle$ of unit length:

$$\min_{|\phi\rangle \in \mathcal{L} + \mathcal{L}^\perp} \langle \zeta | H | \phi \rangle = \langle \eta | H | \eta \rangle = \lambda(H|_{\mathcal{L}}),$$

proving a right-hand side. To show the lower bound on $\lambda(H)$ write any unit vector $|\psi\rangle \in \mathcal{H} = \mathcal{L} + \mathcal{L}^\perp$ as $|\psi\rangle = \alpha|s\rangle + \beta|s^\perp\rangle$ where $|s\rangle \langle s| = \langle s^\perp| s\rangle$ is in $\mathcal{L} \cap \mathcal{L}^\perp$, $\alpha, \beta \in \mathbb{R}$, $\alpha, \beta \geq 0$, and $\alpha^2 + \beta^2 = 1$. So

$$\lambda(H) = \lambda(H_1 + H_2) \geq \alpha^2 \lambda(H_1|s\rangle + \beta \lambda(s)H_1|s^\perp\rangle + \alpha \beta \lambda(s^\perp)H_1|s\rangle + \delta \beta^2.$$ 

For real $H_1$, $|\psi\rangle$, and $|\phi\rangle$:

$$\langle \psi | H_1 | \phi \rangle = \alpha \beta \lambda(s)H_1|s\rangle + \langle s | H_1 | s\rangle = 2\alpha \beta \lambda(s)H_1|s\rangle.$$ 

However, $|s\rangle$ and $|s^\perp\rangle$ are eigenstates of $H_1$ and $\langle s | s^\perp\rangle = 0$, hence

$$\lambda(H_1 + H_2) \geq \lambda(H|_{\mathcal{L}}) + \beta^2(\delta - 2|H_1|).$$

is minimized with $\beta = 0$ so the projection lemma becomes

$$\lambda(H|_{\mathcal{L}}) \leq \lambda(H) \leq \lambda(H_1|_{\mathcal{L}}) \Rightarrow \lambda(H) = \lambda(H_1|_{\mathcal{L}}).$$

APPENDIX B: KARNAUGH MAPS

The Karnaugh map is a tool to facilitate the algebraic reduction of Boolean functions. We made use of this tool in Sec. III during explanation of the specific details required to construct Tables III and IV. Many excellent texts and online tutorials cover the use of Karnaugh maps [28]. This appendix briefly introduces these maps to make the present paper self-contained.

Karnaugh maps (see Fig. 2 for three examples) are organized so that the truth table of a given equation, such as a Boolean equation ($f : \mathbb{B}^n \rightarrow \mathbb{B}$) or multilinear form ($f : \mathbb{B}^n \rightarrow \mathbb{R}$), is arranged in a grid form and between any two adjacent boxes only one domain variable can change value.

This ordering results as the rows and columns are ordered according to Gray code—a binary numeral system where two successive values differ in only one digit. For example, the 4-bit Gray code is given as

$$\{0000, 0001, 0011, 0010, 0110, 0111, 0101, 0100, 1100, 1101, 1111, 1110, 1010, 1011, 1001, 1000\}.$$ 

By arranging the truth table of a given function in this way, a Karnaugh map can be used to derive a minimized function.

To use a Karnaugh map to minimize a Boolean function one covers the 1’s on the map by rectangular coverings containing a number of boxes equal to a power of 2. For example, one could circle a map of size $2^3$ for any constant function $f = 1$. Figures 2(a) and 2(b) contain three circles each—all of two and four boxes, respectively. After the 1’s are covered, a term in a sum of products expression [18] is produced by finding the variables that do not change throughout the entire covering, and taking a 1 to mean that variable $x_i$ and a 0 as its negation. Doing this for every covering yields a function which matches the truth table.

For instance, consider Figs. 2(a) and 2(b). Here the boxes contain simply labels representing the decimal value of the corresponding Gray code ordering. The circling in Fig. 2(a) would correspond to the truth vector (ordered $z_{*}, x_{1}$ then $x_{2}$)

$$(0,0,0,1,0,1,1,1)^T.$$ 

(B1)

The cubes 3 and 7 circled in Fig. 2 correspond to the sum of products term $x_1x_2$. Likewise (5,7) corresponds to $z_{*}x_2$ and finally (7,6) corresponds to $z_{*}x_1$. The sum of products representation of Eq. (B1) is simply

$$f(z_{*}, x_{1}, x_{2}) = x_{1}x_{2} \lor z_{*}x_{2} \lor z_{*}x_{1}.$$ 

Let us repeat the same procedure for Fig. 2(b) by again assuming the circled cubes correspond to 1’s in the functions truth table. In this case one finds $z_{*}$ for the circling of cubes laded (4,5,7,6), $x_2$ for (1,3,5,7), and $x_1$ for (3,2,7,6) resulting in the function

$$f(z_{*}, x_{1}, x_{2}) = x_{1}x_{2} \lor z_{*}x_{2} \lor z_{*}x_{1}.$$ 

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Our use of Karnaugh maps in Sec. III allows one to visualize cube groups (variable products) that are at most two-local in size—the highest order terms realizable with two-local Hamiltonians. In addition, Karnaugh maps help reduce the number of simultaneous equations that, as seen in Sec. III, must be solved—see Eqs. (7) and (8). The Karnaugh maps shown in Figs. 2(a) and 2(b) illustrate groupings for quadratic and linear interactions, respectively, corresponding to two-body terms and one-local fields. In Sec. III, this observation allowed us to derive two-local Hamiltonians and prove which Hamiltonians are not possible to construct given specific numbers of mediator qubits.

[20] It is known that finding the ground state of Hamiltonians formed from simple sums of the inequality operator \( x_i \Leftrightarrow x_j \) is \( NP \) complete on a planar graph [5].
[21] It is understood that a term in a Hamiltonian such as \( \sigma_i \sigma_j \) is the operator \( \sigma \) acting on the \( i \)th and \( j \)th qubit with the omitted identity operator acting on the rest of the Hilbert space. The tensor product symbol \( \otimes \) is omitted between operators.
[25] A simplistic Hamiltonian with vectors in the ground space \( \mathcal{L} \) corresponding to logical AND, that is \( \mathcal{L} = \text{span}[\{000\}, \{010\}, \{100\}, \{111\}] \) (ordered \( |x_1,x_2,x_3\rangle |z_\ast\rangle \), where \( z_\ast = x_1 \Leftrightarrow x_2 \), has the form: \( H = \delta (|000\rangle \langle 000| + |010\rangle \langle 010| - |100\rangle \langle 100| - |111\rangle \langle 111|) \).
[26] For the purpose of this section one is actually only concerned with the null space of the Hamiltonian and the spectral gap \( \delta \) so \( H_{\text{prop}} > |H_{\text{all}}| \) is sufficient.
[27] Assume that \( H_{\text{prop}} \) represents a circuit and is given as an oracle Hamiltonian. One wishes to search for an input bit string \( x \) that will make the circuit output \( z_\ast = 1 \). In this case, we will force an energy penalty any time the circuit outputs 0 by acting on the output qubit, \( z_\ast \), with the Hamiltonian \( H_{\text{all}} = |0\rangle \langle 0| \). After successful adiabatic evolution \( [3,8] \), qubits \( x_1, x_2, \) and \( x_3 \) can be measured to determine an input causing the circuit to output 1. If the circuit never outputs 1, successful adiabatic evolution will return an input that minimizes the Hamming distance from an input that would cause the circuit to output 1.
[29] Where exclusive or (XOR) is given as \( f(x_1,x_2) \overset{\text{def}}{=} x_1 \oplus x_2 = x_1 x_2 + x_1 x_2 = x_1 + x_2 - 2 x_1 x_2 \) and equivalence (EQV) as \( f(x_1,x_2) \overset{\text{def}}{=} x_1 \odot x_2 = x_1 x_2 + x_1 x_2 = 1 - x_1 - x_2 + 2 x_1 x_2 \).
[30] This spectrum corresponds to the Walsh function represented by the eighth column of the matrix \( H^\otimes 3 \), where \( H \) is the \( 2 \times 2 \) Hadamard matrix. We remark that \( \{0,1\} \oplus \wedge \) is the Galois field \( \mathbb{F}_2 \).