Computing Science Group

Ground State Spin Calculus

Jacob D Biamonte

CS-RR-10-13

Oxford University Computing Laboratory
Wolfson Building, Parks Road, Oxford, OX1 3QD

Ground State Spin Calculus

Jacob D Biamonte[1]

[1] *Oxford University Computing Laboratory*[*]

We present an intuitive compositional theory from which one is able to predict and also to control the ground state manifold (and higher energy excitations) of interacting spin systems governed by variants of tunable Ising models, hence giving precise control over the apriori additive structure of Hamiltonian composition. This compositional theory is given in terms of string diagrams: these results were made possible by mapping a variant of the Boolean F2-calculus onto spins and synthesizing modern ideas appearing in Category Theory, Coalgebras, Classical Network Theory and Graphical Calculus. Specifically, we present an algebraic method which allows one to explicitly engineer several energy levels including the low-energy subspace of interacting spin systems. We call this new framework: Ground State Spin Calculus, and in the first instance, the theory requires interactions of up to third order (3-body). By introducing ancillary qubits, we present a novel approach allowing k-body interactions to be captured exactly using only two-body Hamiltonians [Biamonte, Phys. Rev. A 77(**5**), 052331 (2008)]. Our reduction method has no dependence on perturbation theory or the associated large spectral gap and allows for problem instance solutions to be embedded into the ground energy state of Ising spin systems. This could have important applications for future technology as adiabatic quantum evolution might be used to place such a computational system into it's ground state.

[*] `jake@qubit.org`

I. RESULT SUMMARY: EFFECTIVE HAMILTONIAN EMBEDDING OF A NETWORK THEORY

Let's say I gave you a set of vectors, whatever they might be, and that these vectors where all energy eigenstates of some Hamiltonian with tunable coupling terms. Now if I asked you to determine the appropriate settings for each coupling term such that this set of vectors is now the ground state manifold of the Hamiltonian, how would you proceed?

It's a tricky question: due perhaps to the fact that the Hamiltonian has an additive structure. How do we assure that every vector in the selected set and only those vectors are in the span of the ground state?

It turns out that this problem has a very elegant solution. In fact, we're able to map this problem onto string diagrams and hence give it compositional structure. By this we mean that where able to explicitly control which vectors we allow to be in the ground state manifold: this control is done in an intuitive way. Indeed, we recover what appears as and for most purposes behaves like a circuit, and from this circuit we can then recover the Hamiltonian terms and hence the coupling settings that accomplish our task. In this work we will consider the following:

(i): Expose a compositional structure (e.g. a ground state logic) in the span of the ground space of Hamiltonians (see Section II).

(ii): Connect this ground state logic to modern methods in Algebra and Category Theory.

(iii): Ising interactions: The reduction of (i) and (ii) to physical interactions (see Section I E).

These goals (i and ii) provide important steps forward in our understanding of spin systems. In particular, this compositional structure allows us to program Hamiltonians, such that finding any vector in the the span of their ground state solves a computational program of interest (we're able to embed SAT and other NP-complete problems). Now for (ii) above, this is important even outside of quantum theory. By connecting these methods and reductions to modern algebra, we thereby extend existing methods in discrete mathematics concerned with circuits and multi-linear forms. As will be seen, this is done by incorporating such things as bialgebra and Hopf-algebras into the pseudo Boolean forms that can be used to represent Hamiltonians. Let's consider (i) in a bit more detail.

A. Compositional Structure: Ground State Spin Logic (i)

We are able to define logic gates into the span of the ground space of Hamiltonians. By this we mean that we're able to define e.g. the AND-gate in terms of a penalty Hamiltonian, that is a Hamiltonian that adds energy to any vector that is not in the truth table of AND:

$$H_{\mathsf{AND}} = \delta(\mathbb{1} - |000\rangle\langle 000| - |010\rangle\langle 010| - |100\rangle\langle 100| - |111\rangle\langle 111|) \tag{1}$$

Here the Hamiltonian acts on three spins, and δ is a large positive constant. A quick check shows that the third spin is indeed a function of the first two: this function is Boolean AND (see also 11). The ground states (e.g. zero energy eigenspace)

$$\text{span}\{|000\rangle, |010\rangle, |100\rangle, |111\rangle\} \tag{2}$$

where the excited δ energy subspace is given as

$$\text{span}\{|001\rangle, |011\rangle, |101\rangle, |110\rangle\} \tag{3}$$

Now to use the Hamiltonian induced gate, we simply add additional terms. These additional terms are added to set the input qubits to certain values. Say we add a penalty $|0\rangle|0\rangle$ on both of the first two qubits (spins 1 and 2): this sets them both to $|1\rangle$. Another quick check reveals that the third qubit is now in state $|1\rangle$. If on the other hand we where to add the penalty $|1\rangle|1\rangle$ to the output qubit (spin 3) of our Hamiltonian induced ground state logic gate, the inputs would be in the span of the following vectors:

$$\text{span}\{|00\rangle, |01\rangle, |10\rangle\} \tag{4}$$

corresponding precisely to input values needed to make the logic AND-gate output zero. So this enables one to operate circuits *backwards*, or in actuality, any direction one wishes, as temporal ordering is for these purposes irrelevant here. Of course, setting an energy penalty to the output of a logic circuit in such a way thereby enables us to solve NP-hard problems (for details see 12).

This method enables us to several interesting things: importantly, we're now able to define a graphical language to represent Hamiltonian ground states. Hence we're now able to turn the additive structure of Hamiltonian ground states into a compositional structure: given by circuits. This is in fact an instance of the same graphical language we have considered in other work: Categorical Tensor Network States!

B. From Low-Energy Hamiltonians to Diagrammatic Laws: The linear fragment (ii.1)

The theory of Categories provides a framework to elevate diagrammatic reasoning to a rigorous tool — e.g. proofs can be done graphically! We can leverage this framework to define the algebraic operations we will represent as Hamiltonian penalties in this work, and this definition will be done graphically.

Remark 1 (Graphical Calculus)**.** *The graphical calculus used in the present diagrams is based on a so called Penrose-Joyal-Street calculus. This in turn is based largely on a completeness result (originally proved by Joyal and Street in Theorem 2.3 of [1] see also [2]) about the kinds of string diagrams that inspire parts of this work. See also the work on Categorical Quantum Theory [3] and Selinger's survey of graphical languages for monoidal categories (these are the categories which describe Hilbert spaces and quantum theory [4]).*

To get an idea of how the calculus will work, consider Figure 1, which forms a presentation of the linear fragment of the F2 or Boolean calculus: that is, the calculus of Boolean algebra, restricted to the building blocks that can be used to generate linear Boolean functions.

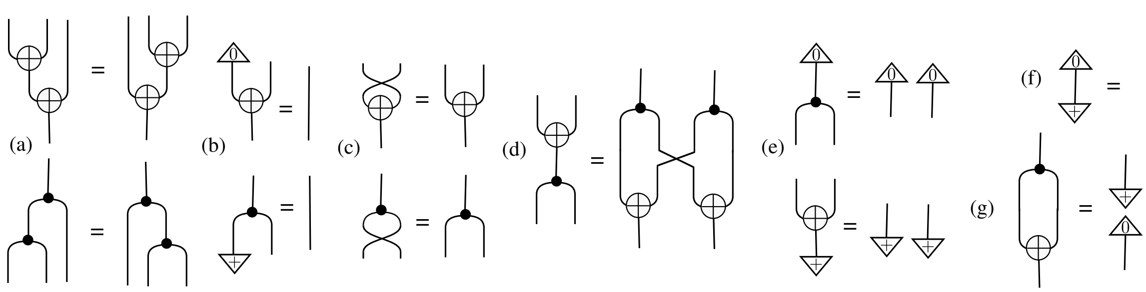


FIG. 1. Read top to bottom. A presentation of the linear fragment of the F2 calculus. The plus ($\oplus$) dots are XOR and the black ($\bullet$) dots represent COPY. For instance, (d) represents the bialgebra law and (g) the Hopf-law (in this case true as $x \oplus x = 0$). In the present work, we map this graphical calculus (save g) onto the ground states of spin Hamiltonians.

It turns out that all of these have a controllable representation on the ground state manifold of commuting Hamiltonians, except (g). The left hand side of (g) maps a spin to $|0\rangle$ by applying the penalty $|1\rangle\langle 1|$ whereas in this work we have interpreted the plus triangle as applying the identity Hamiltonian — e.g. the trivial spin penalty corresponding to span$\{|0\rangle, |1\rangle\}$.

What's all this mean in terms of spins? Well, if we consider (a) in Figure 1, associativity means that the effective ground state of a Hamiltonian can be replaced (interchangeably) as shown in Figure 2.

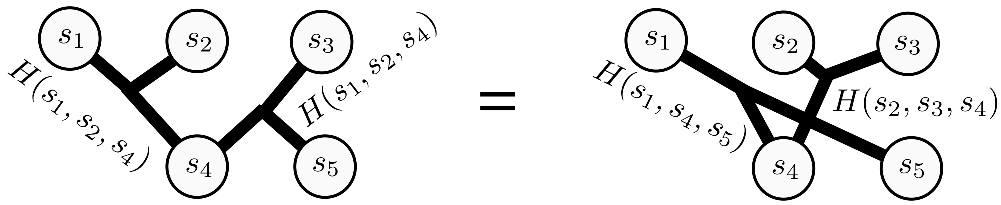


FIG. 2. Associativity condition on two Hamiltonians acting on five spins. The effective Hamiltonians acting on the ground state can be interchanged, hence $H(s_1, s_2, s_4) + H(s_4, s_3, s_5) =$.

The higher levels my not behave this way, but we're only concerned at this stage with the ground state manifold (we consider constructing higher energy subspaces in Section VI).

Example 2 (The miracle of ground state Hopf Algebra)**.** Let us consider a pair of Hamiltonians, H_{COPY} and $H_\oplus$ defined as

$$H_{\mathsf{COPY}} = \delta(\mathbf{1} - |000\rangle\langle 000| - |111\rangle\langle 111|) \tag{5}$$

$$H_\oplus = \delta(\mathbf{1} - |001\rangle\langle 001| - |110\rangle\langle 110| - |010\rangle\langle 010| - |101\rangle\langle 101|) \tag{6}$$

We can map these onto boolean variables, setting $\delta = 1$ and allowing the Hamiltonians to interact on spins labeled $3, 4$ (see Figure 3) leads to the expressions

$$H_{\mathsf{COPY}}(x_3, x_4, x_6) = \frac{1}{4}(3 - x_4x_6 - x_3(x_4 + x_6)) \tag{7}$$

$$H_\oplus(x_2, x_3, x_4) = \frac{1}{2}(1 + x_2x_3x_4) \tag{8}$$

Now we want to explore, the effective Hamiltonian acting on the low-energy sector. We have

$$H_{\mathsf{COPY}}(x_3, x_4, x_6) + H_\oplus(x_2, x_3, x_4) = \frac{1}{4}(5 + (-1 + 2x_2)x_3x_4 - (x_3 + x_4)x_6) \tag{9}$$

and hence strong coupling between spins 3 and 4. It's a miracle however, that the ground state decouples into product states! Spin 2 is forced to $|0\rangle$ whereas the other spins are free (e.g. span$\{|0\rangle, |1\rangle\}$). The effective low energy Hamiltonians hence satisfy the Hopf-law, and hence can be safely interchanged if one is concerned with the low-energy sector, which is most often the case. (We note that we pin-down the specifics on the level splitting δ in Section III).

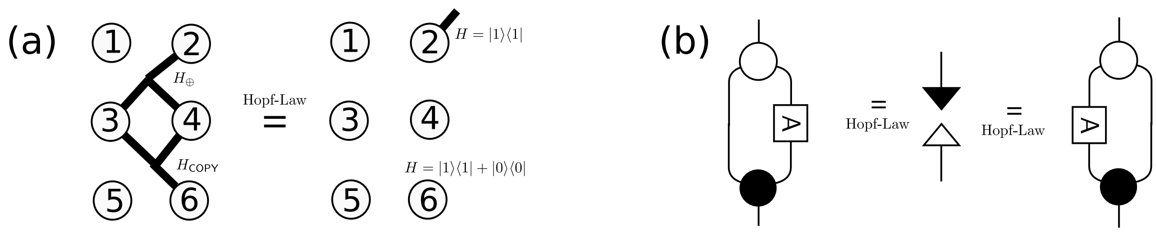


FIG. 3. (a) Hopf-law satisfied in the effective ground state Hamiltonian. In the effective Hamiltonians acting on the ground state, the spins become completely decoupled, allowing for the replacement $H_{\mathsf{COPY}}(x_3, x_4, x_6) + H_\oplus \mapsto |1\rangle\langle 1|_2$. (b) The standard presentation of the Hopf-law with antipode A — here the antipode is assumed to be trivial $A = \mathbf{1}$.

C. Graphical Hamiltonian Reductions: universality and bialgebras (ii.2)

As we have mentioned, the excited states of the Hamiltonians don't always satisfy the same diagrammatic laws as the low-energy effective subspace. The miracle however, happens in the low-energy subspace: this is the effective Hamiltonian acting on the low-energy subspace, which is the only subspace of interest for most applications. We're able to make this reductions without perturbation theory, since we don't have level mixing, we can replace those higher energy level terms with terms that satisfy diagrammatic laws (e.g. Hopf-law) as we're only concerned with the ground state.

To recover the full F2-calculus, one must consider a non-linear Boolean Hamiltonian-gate: in our case, we use the AND-Hamiltonian we have defined above (1). One will then arrive at a full presentation of F2 by considering Figure 1 together with Figure 4 form a full presentation of F2 [5]. In this work, we will give the F2-calculus a representation (on ground spin states). Again, we're able to give all of these equation vivid meaning in the ground state manifold of a spin Hamiltonian save (g) — we don't loose much, if anything: it's the matter of us interpreting the plus triangle as the identity spin penalty: span$\{|0\rangle, |1\rangle\}$.

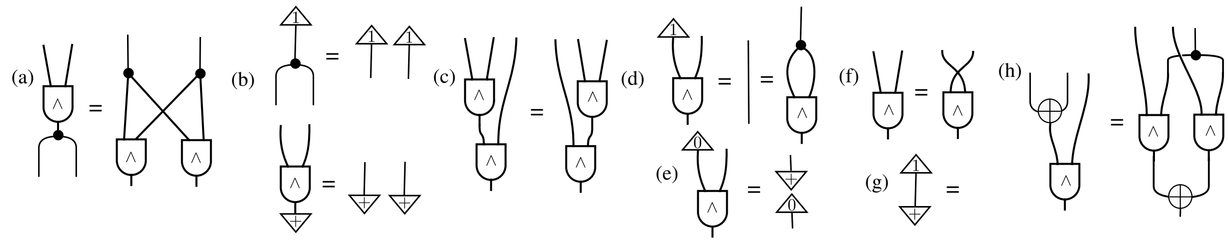


FIG. 4. Read top to bottom. A presentation of the F2-calculus with Figure 1. For instance, (h) represents distributivity of $\mathsf{AND}(\wedge)$ over XOR $(\oplus)$, and (d) shows that $x \wedge x = x$. Each of these has a vivid interpretation in the low-energy effective Hamiltonians we consider in this work, save (g).

Remark 3 (Full Set of Defining Equations)**.** *We note that the presentations in Figure 1 together with Figure 4 are not just a set of relations and identities on circuit components, but instead represent a complete set of defining equations.*

Example 4 (Another miracle: ground state effective bialgebra)**.** As a concluding example, we consider how the bialgebra law can be satisfied in the effective low-energy sector of a Hamiltonian. This is illustrated with H_{COPY} and $H_\oplus$ in Figure 5.

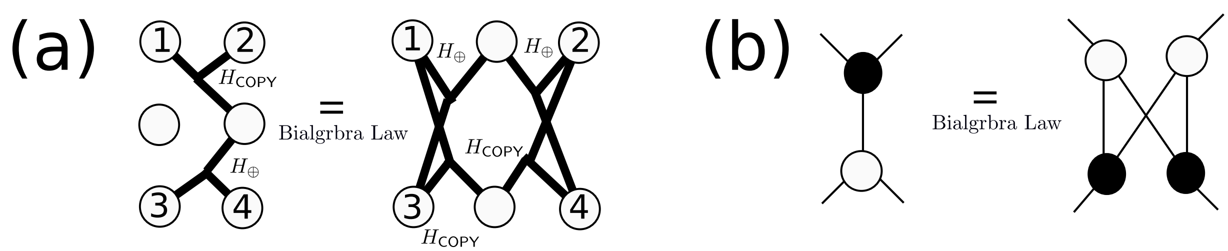


FIG. 5. (a) Hopf-law satisfied in the effective ground state Hamiltonian. (b) The standard presentation.

D. Ising interactions: The reduction to physical interactions (iii)

The logic gates we have mentioned above, define 3-body interactions, but real life Hamiltonians are typically 2-body. It turns out that we are in fact able to do a type of reduction, which allows us to embed these 3-body interactions into the ground space of 3-body Hamiltonians, this is done by adding extra qubits.

E. The k-body into two-body Hamiltonian embedding problem

We have sketched an elegant framework to reason over the ground state manifold induced in the low-energy effective subspace of spin Hamiltonians. This framework requires three-body interaction, but Hamiltonians that exist in nature are typically limited to two-body interactions. Indeed, given a Hamiltonian comprised solely of 1-body and 2-body terms, from this Hamiltonian, and with the aid of ancillary qubits, how might one 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 [6–10] or the equivalent computational task of determining the ground state [10–12].

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 [6, 11]. The extension to quantum complexity classes was prompted when Kitaev [12], inspired by ideas from Feynman [13], showed that the ground state energy problem of the 5-local (that is, 5-body) random field quantum spin model was complete for the quantum analogue of the class NP. Thus it was shown that 5-local Hamiltonian was QMA-complete and the quest to determine the complexity of various spin models began [14–21].

Ideas from the theory of quantum computation have also led to the use of ground state properties of quantum systems for computation [8, 22, 23]. This is known as the adiabatic model of quantum computation [8, 22] — 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.

Kitaev's result later inspired proof of the polynomial equivalence between quantum circuits and adiabatic evolutions [23] as well as proofs of the QMA-completeness of 3-local Hamiltonian [14, 15]. Kempe, Kitaev and Regev subsequently proved the QMA-completeness of Hamiltonians formed from linear combinations of the two letter words taken from the sigma alphabet $\Sigma \stackrel{\text{def}}{=} \{\mathbb{1}, \sigma^x, \sigma^y, \sigma^z\}$ [16]. Oliveira and Terhal then proved the QMA-completeness of Hamiltonians formed from this alphabet acting on subgraphs of the 2D square lattice [17]. In [18] the QMA-completeness of quantum spin models with relatively simple interactions between spins was finally shown. For instance, the model Hamiltonian

$$H_{\mathrm{ZZXX}} = \sum_i h_i \sigma_i^z + \sum_i \Delta_i \sigma_i^x + \sum_{<i,j>} J_{ij} \sigma_i^z \sigma_j^z + \sum_{<i,j>} K_{ij} \sigma_i^x \sigma_j^x \tag{10}$$

was shown to be QMA-complete [18]. More recently, the QMA-completeness of D-dimensional quantum spin chains for the case of D=12 and 13 was demonstrated [20, 21]. Proving the QMA-completeness of problems other than LOCAL HAMILTONIAN has been accomplished — such as the N-REPRESENTABILITY problem [19].

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 2-body terms [16–18]. 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.

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 2-body interactions; under the restriction that all terms in the Hamiltonian share the same basis.

F. Manuscript Structure

The remainder of this paper begins with an introduction to Spin Calculus in II, followed by Section III. This section outlines the ground state calculus first for single spins, then spin pairs and finally explains how the ground states of 3-body Hamiltonians can be used to embed any Boolean function (and for that matter, any switching circuit). We present a summary of the network composition of ground state logic gate Hamiltonians in Section IV A. We then proceed to discuss the effective ground state algebra properties, such as Bialgebra and Hopf algebra. Section V reduces the 3-local Hamiltonians used in Section III to the case of 2-local Hamiltonians: In addition, we prove Theorem 21, which states the existence of an efficient method to construct Hamiltonians that simulate Boolean functions containing k-variable couplings (i.e. $x_1 \wedge x_2 \wedge \cdots \wedge x_k$). In Section VI we construct 2-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 VI also contains a proof of Theorem 27, 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 [14, 16, 23]. 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 [12, 14] as well as that for discrete functions and circuits [24, 25].

II. INTRODUCING SPIN CALCULUS

It is convenient to think of a spin as a bi-state system that can point up ($|0\rangle$) or down ($|1\rangle$). In a system of n interacting spins, each configuration of spin orientations (i.e. one of 2^n eigenvectors $\{|0\rangle, |1\rangle\}^n$) has an associated energy (i.e. one of 2^n possibly degenerate eigenvalues $\{E_0, E_1, ..., E_N\}$). This energy is governed by the Hamiltonian operator — a Hermitian matrix. We will proceed to detail the building blocks of calculus we have developed to reason about the low-energy sector of spin Hamiltonians.

A. Ground States of Single Spins

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 combinations of operators taken from the set

$$\{\mathbb{1}, \pm\sigma\}, \tag{11}$$

where the identity operator ($\mathbb{1}$) can be scaled to ensure positive-semidefiniteness and the operator σ has eigenvectors $|0\rangle$ and $|1\rangle$ with respective eigenvalues $+1$ and -1. The energy levels of the Hamiltonian operator $\frac{1}{2}(\mathbb{1}+\sigma_i)$ $\left(\frac{1}{2}(\mathbb{1}-\sigma_i)\text{ respectively}\right)$ corresponding to the states $|0\rangle$ and $|1\rangle$ are 1 and 0 (0 and 1 respectively). Addition of the operator $\frac{1}{2}(\mathbb{1}+\sigma_i)$ $\left(\frac{1}{2}(\mathbb{1}-\sigma_i)\right)$ adds an energy penalty to the state $|0\rangle$ ($|1\rangle$) and can be thought of as negation (assignment) of variable x_i.

Remark 5 (Summary of Single Spin Operations and Diagrammatics)**.** *Bit assignment corresponds to mapping the identity Hamiltonian (*$\text{span}\{|0\rangle, |1\rangle\}$*) to either logical-zero (*$\text{span}\{|0\rangle\}$*) or logical-one (*$\text{span}\{|1\rangle\}$*). In the diagrammatic language, we can represent the identity Hamiltonian on a spin as simply an unaltered dot representing a spin, or by placing a plus-state triangle in the network diagram (this adheres to some degree with notation from work on Categorical Quantum Circuits). Likewise, bit assignment is given by placing a triangle on the spin in the network diagram representing the Hamiltonian system (see examples in Figure 6).*

FIG. 6. (a) We denote the identity Hamiltonian acting on a single spin (labeled 1) by either an unaltered single spin, or with the attached triangle with a + in the center denoting $\text{span}\{|0\rangle, |1\rangle\}$. In (b) the spin labeled (1) is acted on by the penalty Hamiltonian, setting the ground state to $|0\rangle$. This is denoted with the triangle denoting $\text{span}\{|0\rangle\}$. We don't discriminate in placing the direction of the triangle on spins.

B. Ground States of Spin Pair Interactions

In the case of two Ising spins, a complete basis of configurations are $|00\rangle, |01\rangle, |10\rangle$ and $|11\rangle$. Let us add scaled sums of a coupling term to our Hamiltonian: $\pm\sigma_i\sigma_j$. One can think of adding the operator

$$H_{\Leftrightarrow} \stackrel{\text{def}}{=} \frac{1}{2}(\mathbb{1}-\sigma_i\sigma_j) \tag{12}$$

as a logical equality operation (i.e. the characteristic function $x_i \Leftrightarrow x_j$ is true) and the operator

$$H_{\not\Leftrightarrow} \stackrel{\text{def}}{=} \frac{1}{2}(\mathbb{1}+\sigma_i\sigma_j) \tag{13}$$

as a logical inequality operation (i.e. $x_i \not\Leftrightarrow x_j$ is true) between spins. For example, assume we act on a dual spin system with the Hamiltonian for inequality: the ground space is in span$\{|01\rangle, |10\rangle\}$, so any vector that corresponds to two spin variables being equal — e.g.

$$\text{span}\{|11\rangle, |00\rangle\} \stackrel{\text{def}}{=} \text{span}\{|x\rangle|y\rangle | x = y, \forall x, y \in \{0, 1\}\} \tag{14}$$

receives an energy penalty.

Example 6 (Summary of Two Spin Operations and Diagrammatics)**.** In this subsection spin-wise interactions representing equality and inequality were given. In the graphical language, we represent equality between spins with simply a wire. A wire connecting n-spins has ground state in span$\{|0...0\rangle, |1...1\rangle\}$. One may be familiar with these wires from classical digital circuits, or in string diagrams (e.g. snake equations). Inequality operations are given by placing the symbol for inverter (or NOT) on the wire connecting spins. This is summarized in Figure 7.

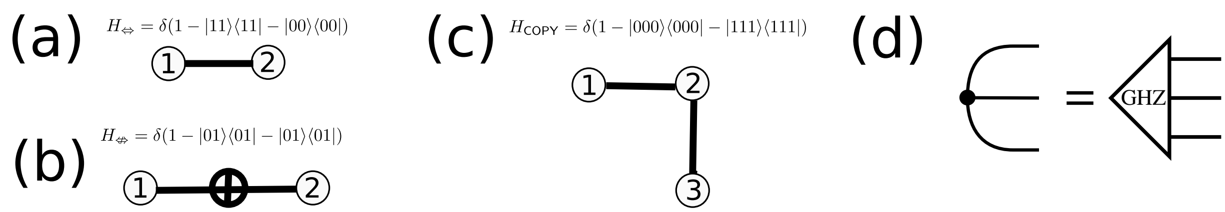


FIG. 7. (a) Equality between two spins is given simply as a wire. It is common in our notation to also omit the circles representing spins. (b) Inequality between spins is given by a wires with an inverter symbol. (c) Multiple equality operators can from the familiar COPY operation (d) Readers may recognize the notation for COPY as a GHZ-state. We note that that each wire can represent 1 to n-spins (see 9).

C. Towards Universal Gates: Ground States of Three Interacting Spins

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 (see Remark 7). This will be done next, in Section III and V, 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 arity operations require at least three spins as $x_i \square x_j = z_\star$. What we need is to find a way to set the low-energy subspace of three spins s_i, s_j and $z_\star$ to be, for instance, the logical AND of the spins $s_i \wedge s_j = z_\star$. 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 (see Remark 8):

$$H_{\text{Ising}} = \sum_i h_i \sigma_i + \sum_{\langle i,j \rangle} J_{ij} \sigma_i \sigma_j. \tag{15}$$

Impressive demonstrations using qubits based on Josephson junctions [26–28] make an adiabatic [8, 22] realization of ground state logic gates using variants of the Hamiltonian (15) a foreseeable possibility.

Remark 7 (Complexity of the Ground State Energy Problem)**.** *It is known that finding the ground state of Hamiltonians formed from simple sums of the inequality operator* $x_i \not\Leftrightarrow x_j$ *(see Figure 7 b) is* NP*-complete on a planar graph [11].*

Remark 8 (Tensor Product Notation)**.** *It is understood that a term in a Hamiltonian such as* $\sigma_i \sigma_j$ *is the operator* σ *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.*

Remark 9 (Outlining the graphical language)**.** *The graphical language we work with looks and behaves for most purposes like one would expect from circuits. There are a few minor advantages that we experience, as temporal ordering can be relaxed in our case. To summarise, wires are replaced with one to* n *spins acted on by equality Hamiltonians (mapping the ground state to e.g.* $\text{span}\{|0\rangle, |1\rangle\}$ *to* $\text{span}\{|0...0\rangle, |1...1\rangle\}$*). Inverters (*$\mathsf{NOT}$*-gates) are replaced with inequality Hamiltonians. Gates are replaced with 3-body interactions as shown in Figure 8.*

Remark 10 (Recent and Related Work)**.** *The ideas of using ground states to compute has had recent growing interest [10, 29–31]. In particular, recent work by Crosson, Bacon and Brown [29] considered fault tolerance of the ground state model. Ground state logic gates were also defined and used in recent work [30, 31].*

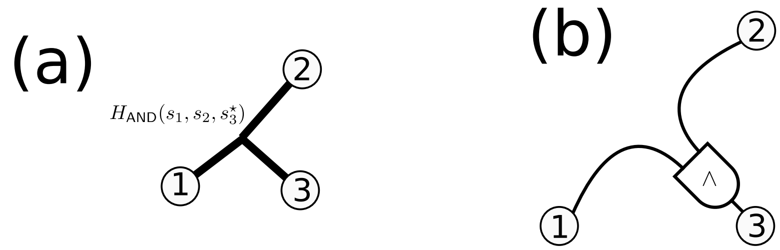


FIG. 8. (a) Conceptual depiction of three-spins being acted on by the Hamiltonian that applies the AND-penalty: $H_{\mathsf{AND}} = \delta(\mathbb{1} - |000\rangle\langle 000| - |010\rangle\langle 010| - |100\rangle\langle 100| - |111\rangle\langle 111|)$ resulting in the ground state being in span$\{|000\rangle, |010\rangle, |100\rangle, |111\rangle\}$. (b) The depiction in the graphical language.

III. COMPOSITIONAL STRUCTURE: 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 $\Pi_\mathcal{L} \stackrel{\text{def}}{=} (\mathbb{1} - \mathcal{L})$ be defined as a projector onto $\mathcal{L}$. Then $\Pi_\mathcal{L} H \Pi_\mathcal{L}$ is the restriction of H to the subspace $\mathcal{L}$ — let us write this restriction as $H|_\mathcal{L}$.

To develop the logic, consider the Hamiltonian H_{prop} such that $H_{\text{prop}}|_\mathcal{L} = 0$ and $H_{\text{prop}}|_{\mathcal{L}^\perp} \geq \delta$ $(> 2\|H_{\text{in}}\|)$ were H_{in} is a perturbation later used to set the circuits inputs, the norm $\|\cdot\|$ is the magnitude of the Hamiltonians largest eivenvalue and δ is the spectral gap between the $\mathcal{L}^\perp$ and $\mathcal{L}$ subspaces. We are faced with the task of ensuring that $H_{\text{prop}}|_\mathcal{L}$ is a zero eigenspace when $\mathcal{L}$ spans the truth table of the logical operation of interest, e.g.

$$\mathcal{L} = \text{span}\{|x_1\rangle|x_2\rangle|x_1 \Box x_2\rangle | \forall x_1, x_2 \in \{0,1\}\}. \tag{16}$$

Let $\mathcal{L}$ be the low-energy subspace representing the truth table in the binary observables. Explicitly, in the case of logical AND,

$$\mathcal{L} = \text{span}\{|000\rangle, |010\rangle, |100\rangle, |111\rangle\} \tag{17}$$

(ordered $|x_1 x_2\rangle|z_\star\rangle$, where $z_\star = x_1 \wedge x_2$), which is a zero eigenspace of H_{prop} and

$$\mathcal{L}^\perp = \text{span}\{|001\rangle, |011\rangle, |101\rangle, |110\rangle\} \tag{18}$$

$(z_\star \neq x_1 \wedge x_2)$ will be all eigenspaces of at least δ.

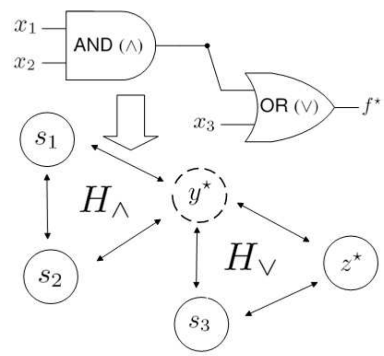


FIG. 9. Illustrating the mapping between circuits (with boolean variables x_i) and spins (s_i) for the example given in (21). One can use any number of methods to embed logical networks [24] into the ground space of Hamiltonians.

Example 11 (3-body ground state AND-gate)**.** A simplistic Hamiltonian with vectors in the ground space $\mathcal{L}$ corresponding to logical AND, that is $\mathcal{L} = \text{span}\{|000\rangle, |010\rangle, |100\rangle, |111\rangle\}$ (ordered $|x_1 x_2\rangle|z_\star\rangle$, where $z_\star = x_1 \wedge x_2$), has the form:

$$H_{\mathsf{AND}} = \delta(\mathbb{1} - |000\rangle\langle 000| - |010\rangle\langle 010| - |100\rangle\langle 100| - |111\rangle\langle 111|) \qquad (19)$$

See also Section IV A and Table 10.

One can add a perturbation, H_{in}, to set the circuits inputs. We will write this as a projector onto the n long binary bit vector $\mathbf{x}$. This 1-local projector has the form:

$$\Pi_{\mathbf{x}} \stackrel{\text{def}}{=} |\mathbf{x}^\perp\rangle\langle\mathbf{x}^\perp| = \left(\frac{1}{2}\right)\sum_{i=1}^{n}\left(\mathbb{1} + (-1)^{1-x_i}\sigma_i\right).$$

Now upper bound $\|H_{\text{in}}\|$ (for all two input and single output gates [1]) as $\|H\| \leq 2$. This implies that the spectral gap δ is greater than 2. By noticing that $\forall j, k$

$$H|s_j\rangle = \lambda|s_j\rangle, \qquad H|s_k^\perp\rangle = \lambda|s_k^\perp\rangle$$
$$\text{and} \qquad \langle s_j|H|s_k^\perp\rangle + \langle s_k^\perp|H|s_j\rangle = 0,$$

where $|s_j\rangle \in \mathcal{L}$ and $|s_k\rangle \in \mathcal{L}^\perp$, one recovers the strict equality, $\lambda(H_{\text{in}}|_{\mathcal{L}}) = \lambda(H)$ (see Lemma 14).

[1] For the purpose of this section one is actually only concerned with the null space of the Hamiltonian and the spectral gap δ so $H_{\text{prop}} > \|H_{\text{in}}\|$ is sufficient.

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

$$\mathrm{span}\{|x_1x_2\rangle|y_\star\rangle \mid y_\star = x_1 \wedge x_2, \forall x_1, x_2 \in \{0,1\}\} \tag{20}$$

as $H_\wedge(x_1, x_2, y_\star)$ and, with $y_\star$ defined in (20), write the Hamiltonian with a low-energy subspace in

$$\mathrm{span}\{|x_3y_\star\rangle|z_\star\rangle \mid z_\star = y_\star \wedge x_2, \forall x_3 \in \{0,1\}\}$$

as $H_\wedge(x_3, y_\star, z_\star)$. Then the proposition $x_1 \wedge x_2 \vee x_3 = z_\star$ is constructed as a sum of terms:

$$H = \overbrace{H_\vee(x_1, x_2, y_\star) + H_\wedge(x_3, y_\star, z_\star)}^{H_{\mathrm{prop}}} + H_{\mathrm{in}} \tag{21}$$

and the circuits input, H_{in}, is yet to be defined. The qubit with label $z_\star$ is now equal to $x_1 \wedge x_2 \vee x_3$ and $y_\star$ is a temporary variable that is equal to $x_1 \wedge x_2$, as seen in Table II.

A small perturbation, H_{in}, can be added to set any of the qubits to specified values. For example, to set the input as $x_1 = 1$, $x_2 = 0$ and $x_3 = 0$ one adds the perturbation $H_{\mathrm{in}} = |0\rangle\langle 0|_1 + |1\rangle\langle 1|_2 + |1\rangle\langle 1|_3$ (see also Example 12). If, alternatively, we were to let $H_{\mathrm{in}} = |0\rangle\langle 0|_\star$, which acts on the circuits output $z_\star$, then the low-energy subspace would be spanned by all vectors where the output $z_\star$ is $|1\rangle$. As seen from Table II, this subspace is in

$$\begin{aligned}\mathrm{span}\{&|001\rangle|1\rangle|0\rangle, |011\rangle|1\rangle|0\rangle, |101\rangle|1\rangle|0\rangle,\\ &|110\rangle|1\rangle|1\rangle, |111\rangle|1\rangle|1\rangle\},\end{aligned}$$

where we adhere to the ordering $|x_1x_2x_3\rangle|z_\star\rangle|y_\star\rangle$. If instead we were to add the perturbation H_{in} to the qubit labeled $|y_\star\rangle$, the ground space would be spanned by $\{|110\rangle|1\rangle|1\rangle, |111\rangle|1\rangle|1\rangle\}$.

Example 12 (Adiabatic Ground State Logic Gates)**.** Assume that H_{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 $z_\star = 1$. In this case, we will force an energy penalty any time the circuit outputs 0 by acting on the output qubit, $z_\star$, with the Hamiltonian $H_{\mathrm{in}} = |0\rangle\langle 0|_\star$. After successful adiabatic evolution [8, 22], 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.

To complete our reduction, the 3-local Hamiltonians, just described, will be reduced in the next section to 2-local Hamiltonians. Before continuing to our 2-local reduction, let us state Lemma 14 and Theorem 13 — the proof of which is implied by the results of this section. Here we choose a finite set Ω of one-output Boolean functions as basis. Then, an Ω-circuit works for a fixed number of Boolean input variables and consists of a finite number of gates, where each gate is defined by it's type taken from Ω. (For additional background information on boolean functions and switching circuits see the freely available standard reference [24].)

Theorem 13 (Boolean Ground States). *Let f be a switching function given as the map $f : \{0,1\}^k \to \{0,1\}^m$ for finite k and m. Now let there be an asynchronous Ω-circuit computing f. Then there exists an Ω-circuit embedding into the ground space of a 3-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 Ω-circuit, as well as k and m. ii.) The Ω-circuit embedding is upper bounded by a number of qubits $\mathcal{O}(1)$-reducible to the number of classical gates required on the same lattice. (See also Section IV A and Table 10.)*

An important technical tool used in our construction is a variant of the projection Lemma [14, 16, 23] — 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 $\mathcal{L} \in \mathcal{H}$ 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 δ $(> 2\|H_1\|)$. 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 $\lambda(H_1|_\mathcal{L})$. Thus, by adding H_2 one adds a penalty (proportional to δ) to any vector in $\mathcal{L}^\perp$. To state the Projection Lemma (Strict Equality) we:

Lemma 14 (Projection Lemma). *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 $\mathcal{L} = \mathrm{span}\{|s_j\rangle|\forall j\}$ and $\mathcal{L}^\perp = \mathrm{span}\{|s_k^\perp\rangle \forall k\}$ for finite j, k. Consider the restriction $H_2|_\mathcal{L} = 0$ and $H_2|_{\mathcal{L}^\perp} \geq \delta(> 2\|H_1\|)$. Then, if $\forall j, k$ $H|s_j\rangle = \lambda|s_j\rangle$ $(\forall k\ H|s_k^\perp\rangle = \lambda|s_k^\perp\rangle)$, $\langle s_j|H|s_k^\perp\rangle + \langle s_k^\perp|H|s_j\rangle = 0$ the following equality holds: $\lambda(H) = \lambda(H_1|_\mathcal{L})$.*

IV. GROUND STATE ALGEBRAS ON SPINS

In this section we will outline some key and interesting properties of how the ground state penalty Hamiltonians we define in this work interact. We will continue by outlining penalties to define the standard Boolean functions into the span of the ground state energies.

A. Summarizing: Network Composition of Ground State Logic Gate Hamiltonians

In classical computer science, a universal set of gates, is able to express any n-bit Boolean function

$$f : \mathbb{B}^n \to \mathbb{B} :: (x_1, ..., x_n) \mapsto f(x_1, ..., x_n) \tag{22}$$

Universal sets include {COPY, NAND}, {COPY, AND, NOT}, {COPY, AND, XOR,1}, {OR, XNOR,1} and others. We captured this in Theorem 13. In the following Table (10) we illustrate the three-body Hamiltonian penalties that force the span of the ground state to represent classical switching functions of two-inputs [32].

non-linear	linear (Frobenius Algebras)
$H_{\mathsf{AND}} = \delta(\mathbf{1} - \vert 000\rangle\langle 000\vert - \vert 010\rangle\langle 010\vert - \vert 100\rangle\langle 1000\vert - \vert 111\rangle\langle 111\vert)$	
$H_{\mathsf{OR}} = \delta(\mathbf{1} - \vert 001\rangle\langle 001\vert - \vert 011\rangle\langle 011\vert - \vert 101\rangle\langle 101\vert - \vert 111\rangle\langle 111\vert)$	$H_{\mathsf{XOR}} = \delta(\mathbf{1} - \vert 000\rangle\langle 000\vert - \vert 011\rangle\langle 011\vert - \vert 101\rangle\langle 101\vert - \vert 110\rangle\langle 110\vert)$
$H_{\mathsf{NAND}} = \delta(\mathbf{1} - \vert 001\rangle\langle 001\vert - \vert 011\rangle\langle 011\vert - \vert 101\rangle\langle 101\vert - \vert 110\rangle\langle 110\vert)$	$H_{\mathsf{XNOR}} = \delta(\mathbf{1} - \vert 001\rangle\langle 001\vert - \vert 010\rangle\langle 010\vert - \vert 100\rangle\langle 100\vert - \vert 111\rangle\langle 111\vert)$
$H_{\mathsf{NOR}} = \delta(\mathbf{1} - \vert 001\rangle\langle 001\vert - \vert 010\rangle\langle 010\vert - \vert 100\rangle\langle 100\vert - \vert 110\rangle\langle 110\vert)$	

FIG. 10. The bit patterns encoded in the span of the ground state represent Boolean function (given by the subscript on H) such that the right most bit is the Boolean functions output, and the two left bits are the functions inputs, and the non-linear Boolean functions are on the left side of the table and the linear functions on the right.

B. Associativity, Distributivity and Commutativity.

The penalty Hamiltonians we have considered (Figure 10) embed boolean functions which are associative and commutative. As *products*, AND, XOR and COPY are associative, unital (that is they have units, $|1\rangle$, $|0\rangle$ and $|+\rangle$ respectively) commutative algebras. This was already expressed diagrammatically in Figures 1 (a) and 4 (c).

As ground states, one is able to embed and couple higher order (greater than two-body) interactions (that is, products) into the ground energy states of spin systems. The associativity law for AND and XOR are given as:

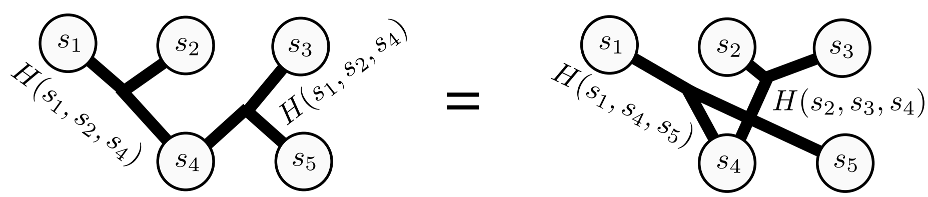
$$(x_1 \wedge x_2) \wedge x_3 = x_1 \wedge (x_2 \wedge x_3) \tag{23}$$

$$(x_1 \oplus x_2) \oplus x_3 = x_1 \oplus (x_2 \oplus x_3) \tag{24}$$

Both now have evident meaning in terms of the effective Hamiltonian interaction in the low-energy subspace. In these equations, as Hamiltonian penalties, there will be an extra output spin, which stores the result. Distributivity of AND over XOR then becomes (see (h) in Figure 4)

$$(x_1 \oplus x_2) \wedge x_3 = (x_1 \wedge x_2) \oplus (x_1 \wedge x_2) \tag{25}$$

We of course have commutativity for any product symmetric in it's inputs: this is the case for AND- and XOR-Hamiltonians. The associativity condition on Hamiltonian ground states is given as (see also Figure 2):



C. Ground State Bialgebras

There is a very powerful type of algebra that arises in our setting of Hamiltonian penalties: a bialgebra (See Kassel, Chapter III [33], or [34, 35]). Such an algebra is simultaneously an unital associative algebra (for the associativity condition see (b) in Figure 11)and coalgebra and are characterized by a compatibility condition. In the standard presentation, one considers the following ingredients:

(i): a product (black dot) with a unit (black triangle) see Figure 11 (a)
(ii): a coproduct (white dot) with a counit (white triangle)

precisely, the four compatibility conditions are satisfied if the following holds:

(i): The unit of the black dot is a copy-point of the white dot as in (e) from Figure 11.
(ii): The (co)unit of the white dot is a copy-point of the black dot as in (d) from Figure 11.

(iii): The bialgebra-law is satisfied given in (c) from Figure 11.

(iv): The inner product of the unit (black triangle) and the counit (white triangle) is non-zero (not shown in Figure 11).

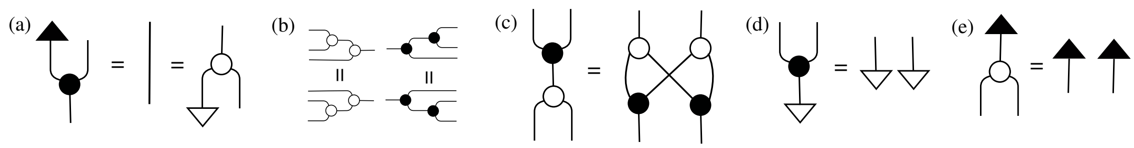
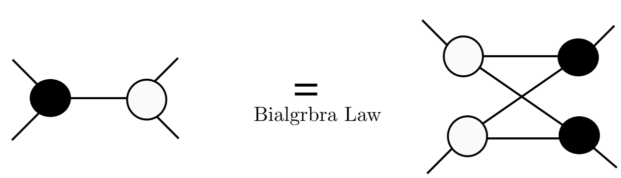


FIG. 11. Bialgebra axioms. (a) unit laws (these are of course left and right units); (b) associativity; (c) bialgebra; (d,e) co-copy points.

Example 15 (Low-energy subspace of H_{COPY}- and H_{AND}-Hamiltonians form Bialgebras)**.** We are in a position to study the interaction of H_{COPY}- and H_{AND}-Hamiltonians. This interaction satisfies the following: (i) the bialgebra law; (ii) the co-copy point of AND is $|1\rangle$; and (iii) the co-interaction with the unit for COPY creates a equality coupling, where an extra bit can then be removed (provided it is involved in no further interactions). See also Figure 1 (a).

Even if two products don't form bialgebras, they can still satisfy the bialgebra condition (and hence not satisfy all of the axioms listed above). For this reason, so we define this law (examples of states that satisfy this law, but are not necessarily bialgebras are given in Example 17

Definition 16 (Bialgebra)**.** A pair of quantum states (black, white below) satisfy the bialgebra law if the following holds:

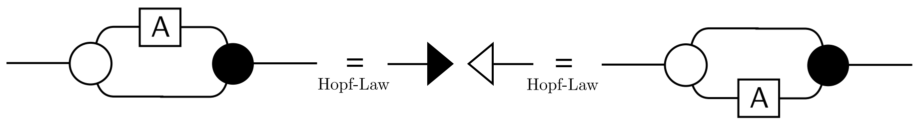


Example 17 (Boolean States from Bialgebras with H_{COPY})**.** The Boolean states, H_{AND}, H_{OR}, H_{XOR}, H_{XNOR}, H_{NAND}, H_{NOR} all satisfy the bialgebra law with H_{COPY}.

D. Ground State Hopf Algebras

A particularly important class of bialgebras are known as Hopf-algebras [34]. This is characterized by the way in which algebras and coalgebras can interact (see Figure 3 a and b). This is captured by the Hopf-law, where linear map A is known as the antipode.

Definition 18 (Hopf-Law)**.** A pair of quantum states satisfy the Hopf-Law if an A can be found such that the following equations hold:



Example 19 (H_{XOR} and H_{COPY} form effective Hopf-algebras in the low-energy subspace)**.** It is well known (see e.g. [5]) that the Boolean gate XOR, satisfies the Hopf-algebra law with trivial antipode with COPY. This indeed holds in the case of Hamiltonian penalties. See also Figure 4 (g).

V. THE K-BODY INTO TWO-BODY REDUCTION

The main result of this section can be found in Table III. To develop this table we used the algebra of multi-linear forms [25] and the Karnaugh map method from discrete mathematics [36] — which we review in Appendix B.

We consider multi-linear forms that are maps f from the Booleans numbers to the reals, where the inputs and outputs are of finite size. For instance, the multi-linear form for AND (OR) is simply $f_\wedge = x_1 \wedge x_2$ ($f_\vee = x_1 + x_2 - 2x_1 \wedge x_2$). Hence, one can express the Boolean equation $f = x_1 \wedge x_2 \vee x_3$ 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:

$$\mathbf{c}^\mathsf{T} = (c_0, c_1, c_2, c_3, c_4, c_5, c_6, c_7,), \tag{26}$$

representing the outputs of a multi-linear function f over the three Boolean input arguments x_1, x_2 and x_3. We wish to construct a canonical representation for any multi-linear function of three variables in terms of the vector $\mathbf{c}$ from (26). We will represent the negation of the variable x as $\bar{x}$ (or using the notational equivalent $\neg x$) and canonically expand (26) as a sum of products:

$$f(x_1, x_2, x_3) = c_0 \cdot \bar{x}_1\bar{x}_2\bar{x}_3 + c_1 \cdot \bar{x}_1\bar{x}_2 x_3 + c_2 \cdot \bar{x}_1 x_2\bar{x}_3 \\ +c_3 \cdot \bar{x}_1 x_2 x_3 + c_4 \cdot x_1\bar{x}_2\bar{x}_3 + c_5 \cdot x_1\bar{x}_2 x_3 \\ +c_6 \cdot x_1 x_2\bar{x}_3 + c_7 \cdot x_1 x_2 x_3. \tag{27}$$

This expansion (27) forms a basis for the space of 3-variable Hamiltonians, but to realize any of the eight terms requires 3-body couplings. This motivates us to write a second canonical expansion, found from a change of variables in (27) and by expanding each term into it's positive polarity form:

$$f(x_1, x_2, x_3) = a_0 + a_1 \cdot x_1 + a_2 \cdot x_2 + a_3 \cdot x_3 \\ + a_4 \cdot x_1 x_2 + a_5 \cdot x_1 x_3 + a_6 \cdot x_2 x_3 \\ + a_7 \cdot x_1 x_2 x_3. \tag{28}$$

This equation (28) also forms a basis for the space of realizable Hamiltonians of 3-spins. In this suggestive form, however, we can truncate (28) past 2^{nd} order and consider the subclass of Hamiltonians that can be realized by setting $a_7 = 0$.

Out of the 16 possible functions of 2-input and 1-output variable, it can be proven that only two are not realizable using 3-spins. These are the 2-local penalty Hamiltonians for XOR ($\oplus$) and XNOR ($\odot$), which are each possible to realize by adding a single mediator qubit (as seen in Table III).

Example 20 (Polynomials for XOR and XNOR)**.** The polynomial for *exclusive* OR (XOR) is given as

$$f_\oplus(x_1, x_2) \stackrel{\text{def}}{=} x_1 \oplus x_2 = \bar{x}_1 x_2 \vee x_1\bar{x}_2 = x_1 + x_2 - 2x_1 \wedge x_2, \tag{29}$$

and *equivalence* (XNOR) as

$$f_\odot(x_1, x_2) \stackrel{\text{def}}{=} x_1 \odot x_2 = \bar{x}_1\bar{x}_2 \vee x_1 x_2 = 1 - x_1 - x_2 + 2x_1 \wedge x_2. \tag{30}$$

We will explain in detail how the positive-semidefinite AND penalty Hamiltonian, $H_\wedge$, is derived. We anticipate that the details of our approach will aid others faced with Hamiltonian constructions. Let $\mathcal{L}$ be the null space of $H_\wedge$ and let all higher eigenspaces

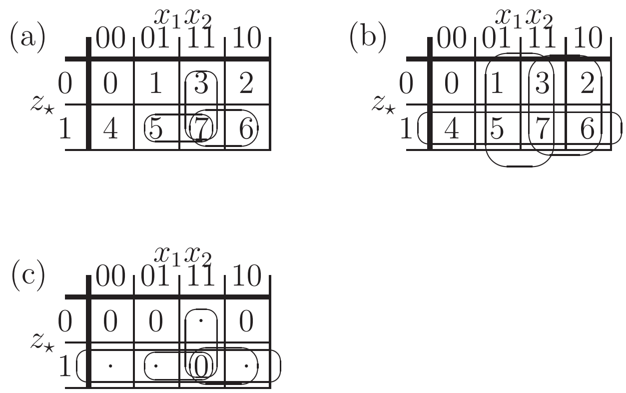


FIG. 12. Karnaugh maps: (a) 2-local (positive polarity) interactions circled (e.g. $q_1x_1x_2+q_2x_1\wedge z_\star+q_3x_2\wedge f^\star$). (b) Linear (positive polarity) fields circled (e.g. $l_1x_1+l_2x_2+l_3x_3$). The interactions in cubes (a) and (b) form a basis for the space of realizable (≤ 3 qubit) positive-definite logical gadget Hamiltonians expressible as: $H(x_1,x_2,z_\star)=k_0+l_1x_1+l_2x_2+l_3x_3+q_1x_1\wedge x_2+q_2x_1\wedge z_\star+q_3x_2\wedge z_\star$, were $\forall i$, $k_0,l_i,q_i\geq 0$. (c) A Karnaugh map illustrating (with ovals) the linear and quadratic terms needed to set the null space of the Hamiltonian (41) to be in span$\{|x_1x_2\rangle|y_\star\rangle|y_\star=x_1\wedge x_2,\forall x_1,x_2\in\{0,1\}\}$.

be given as $\mathcal{L}^\perp$. The penalty Hamiltonian has a null space, $\mathcal{L}$, spanned by the vectors $\{|x_1x_2\rangle|z_\star\rangle|z_\star=x_1\wedge x_2,\forall x_1,x_2\in\{0,1\}\}$. Denote δ as an energy penalty applied to any vector component in $\mathcal{L}^\perp$. Our goal is to develop a Hamiltonian that adds a penalty of at least δ 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 $\mathcal{L}^\perp$.

In order to make the penalty quadratic, one first constructs the Karnaugh map illustrated in Fig. 12 c.) for the case $x_1\wedge x_2=z_\star$. This is done by examining Table I. In the right most column, all possible assignments for the variables x_1, x_2 and $z_\star$ are shown. The Karnaugh map is constructed by examining the second column. Whenever the variable $z_\star$ is not equal to the AND of the variables x_1 and x_2, a penalty of at least δ must be applied, which ensures that vectors in the ground space satisfy $|x_1\rangle|x_2\rangle|x_1\wedge x_2\rangle$. Any vector that must receive an energy penalty of δ is depicted in the Karnaugh map with a dot $(\cdot)$.

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 $z_\star$ must be at least δ — adding the term $p_1z_\star$ to the Hamiltonian, with the constraint $p_1\geq\delta$. Cube 3 must also receive an energy penalty of at least δ, adding the term $p_2x_1\wedge x_2$ to the Hamiltonian $H_\wedge$. With both penalties applied, vectors corresponding to cube 7 must be brought back to the null space — accomplished by subtracting the quadratic energy rewards $r_1 z_\star \wedge x_1$ and $r_2 z_\star \wedge x_2$ from $H_\wedge$. A system of equations for the Hamiltonian $H_\wedge(x_1, x_2, z_\star) =$

$$p_1 z_\star + p_2 x_1 \wedge x_2 - r_2 z_\star \wedge x_1 - r_2 z_\star \wedge x_1 \tag{31}$$

can be solved to set the rewards (r's) and the penalties (p's). This system is derived from the fact that the term $x_1 x_2 x_3$, corresponding to cube 7, must have zero energy: $0 = p_1 + p_2 - r_1 - r_2$ and is subject to the conditions that $p_1, p_2 \geq \delta$ and $|r_1 + r_2| > p_1$. For convenience, let $\delta = 1$ and then determine values for the coefficients in (31) and thus derive the 2-body Hamiltonian (for AND):

$$H_\wedge(x_1, x_2, z_\star) = 3z_\star + x_1 \wedge x_2 - 2z_\star \wedge x_1 - 2z_\star \wedge x_2. \tag{32}$$

If one desires to invert an input variable, she simply applies the transform: $\bar{x}_i \to (1 - x_i)$. For example, the Hamiltonian applying the penalty $H_\wedge(\bar{x}_1, x_2, z_\star)$ is:

$$3z_\star + (1 - x_1) \wedge x_2 - 2z_\star \wedge (1 - x_1) - 2z_\star \wedge x_2. \tag{33}$$

To write this Hamiltonian in terms of spin variables, first change each variable, x_i, to its (matrix) operator form by the replacement $x_i \to |0\rangle\langle 0|_i$. The change to spin variables is then accomplished by the replacement: $|0\rangle\langle 0|_i \to \frac{1}{2}(\mathbb{1} - \sigma_i)$. After these substitutions one arrives at the Hamiltonian (42) which is isomorphic ($\simeq$) to (33).

$$\begin{aligned} & H_\wedge(\bar{x}_1, x_2, z_\star) \simeq H_\wedge(-s_1, s_2, s_\star) = \\ = & \frac{1}{4}(3 + \sigma_1 - \sigma_2 + 2\sigma_\star - \sigma_1\sigma_2 + 2\sigma_1\sigma_\star - 2\sigma_2\sigma_\star) \end{aligned} \tag{34}$$

We now have the necessary machinery in place to state two theorems (21 and 22). In the first, we are concerned with a situation that arises in several applications. That is, one often needs to couple three Boolean variables (AND product), as $x_1 \wedge x_2 \wedge x_3$, using only 2-local Hamiltonians. From our reduction, it is possible to efficiently construct any k-local product term, $x_1 \wedge x_2 \wedge \cdots \wedge x_k$, of this type. We prove this in Theorem 21. We then present Theorem 22, which is a 2-local variant of Theorem 13 — the proof of which follows directly from the results of this section.

Theorem 21 (two-body Embedding of k-body AND-penalty)**.** *Let f_k be a k-local multi-*

x_1	x_2	$z_\star$	$z_\star \stackrel{?}{=} x_1 \wedge x_2$	$H_\wedge(x_1, x_2, z_\star)$
0	0	0	$\langle 000 \vert H_\wedge \vert 000\rangle = 0$	0
0	0	1	$\langle 001 \vert H_\wedge \vert 001\rangle \geq \delta$	3δ
0	1	0	$\langle 010 \vert H_\wedge \vert 010\rangle = 0$	0
0	1	1	$\langle 011 \vert H_\wedge \vert 011\rangle \geq \delta$	δ
1	0	0	$\langle 100 \vert H_\wedge \vert 100\rangle = 0$	0
1	0	1	$\langle 101 \vert H_\wedge \vert 101\rangle \geq \delta$	δ
1	1	0	$\langle 110 \vert H_\wedge \vert 110\rangle \geq \delta$	δ
1	1	1	$\langle 111 \vert H_\wedge \vert 111\rangle = 0$	0

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

linear from and let there be a Hamiltonian H_k acting on the Hilbert space $\mathcal{H}_k$ such that $f_k \simeq H_k$. Then there exists a 2-local multi-linear form, f_2, and corresponding Hamiltonian, H_2, acting on the Hilbert space $\mathcal{H}_2$ (where $\mathcal{H}_k \subseteq \mathcal{H}_2$), with the same low-energy subspace of H_2 in $\text{span}\{|x\rangle|y\rangle | y = f_k(x), \forall x \in \{0,1\}^n, \forall y \in \{0,1\}^m\} \subseteq \mathcal{H}$. *The number of mediator qubits required to realize H_2 is upper bounded by $\mathcal{O}(size(f_k))$. In addition, the spectral gap of H_2 is bounded by the spectral gap of H_k. (See also Example 28.)*

two-body Embedding of k-body AND*-penalty 21.* To construct such a Hamiltonian, we will employ an inductive argument and consider a single (out of w) k-local term, $h_k = x_1 \wedge x_2 \wedge \cdots \wedge x_k$, that couples $k \geq 3$ Boolean variables. We will now show the existence of a 2-local reduction requiring $(k-2)$ mediator qubits to embed h_k into the ground state of a 2-local Hamiltonian. Consider the 2-local coupling $z_\star \wedge x_3$ and add the Hamiltonian that forces an energy penalty whenever $z_\star$ is not the Boolean AND of the variables x_1 and x_2. The 2-local Hamiltonian is written as

$$H_\wedge(x_1, x_2, z_\star) + z_\star \wedge x_3 \simeq \frac{1}{4}(4 - \sigma_1 - \sigma_2 + 3\sigma_\star + \sigma_3 + \sigma_1\sigma_2 - 2\sigma_1\sigma_\star - 2\sigma_2\sigma_\star + \sigma_\star\sigma_3),$$

where $H_\wedge$ is found in Table III, and $z_\star$ is a temporary variable. In words, the variable $z_\star$ is coupled to x_3 and the penalty, $H_\wedge$, forces $z_\star$ 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 $|x_1x_2x_3\rangle$, $\forall i \in \{1,2,3\}, x_i \in \{0,1\}$. For a k-local term $x_1 \wedge x_2 \wedge \cdots \wedge x_k$, this procedure is recursively repeated $k-2$ times. The reduction requires $w(k-2)$ qubits to capture the low-lying eigenspace of H_k with H_2. $\square$

Theorem 22 (Two-body Hamiltonian Penalties for Boolean States)**.** *Let f be a switching function with a fixed number of inputs k and outputs m. Let there be an asynchronous Ω-circuit computing f over the basis $\{\neg, \oplus, \wedge\}$. There exists an Ω-circuit embedding into the ground state of a 2-local Hamiltonian, H_2, such that: i.) The norm of the Hamiltonian $\|H_2\|$ is constant and, in particular independent of the size of f, the Ω-circuit, k as well as m. ii.) The Ω-circuit embedding is upper bounded by a number of qubits $\mathcal{O}(k)$-reducible to the number of classical gates required on the same lattice.*

Theorem 23. *The 2-*LOCAL HAMILTONIAN *problem encompasses* NP*.*

Proof. The $L = L_{yes} \cup L_{no}$ promise problem 2-LOCAL ISING SPIN GLASS $\subseteq$ 2-LOCAL HAMILTONIAN is *loosely* stated as follows [12] (see also [37]): given a finite description of an Ising Hamiltonian (15) acting on a system of n qubits, is the lowest eigenvalue, $\lambda(H_{\text{ISING}})$, at most a (YES instance) or are all eigenvalues of H_{ISING} greater than b (NO instance) such that $b - a > 1/\text{poly}(n)$?

To show that solving the spin glass problem is at least as hard as solving any other problem in NP, one will embed a classical Ω-circuit into the null space of H_{ISING}. We will show that knowledge of the promise

$$\underbrace{\lambda(H_{\text{ISING}}) \leq a}_{L = L_{yes}} \qquad \text{vs.} \qquad \underbrace{\lambda(H_{\text{ISING}}) > b}_{L = L_{no}}$$

is equivalent to verifying solutions of an NP-complete problem, such as k-SAT (cf. [24]).

Consider an Ω-circuit with input x that is upper bounded in size by $\mathcal{O}\left(\text{poly}(|x|)\right)$. Denote H_{prop} as a 2-local Hamiltonian which assures that the null space is spanned by the truth table representing the Ω-circuit — let this null space be denoted as $\mathcal{L}$ and the orthogonal compliment as $\mathcal{L}^{\perp}$. Let us now set the input, x, of the Ω-circuit contain the proof $x_1 ... x_n$. This is done by adding the penalty $H_{\text{in}} = \left(\frac{1}{2}\right) \sum_{i=1}^{n} \left(\mathbb{1} + (-1)^{1-x_i} \sigma_i\right)$ which acts on the n inputs. Now the null space of the Hamiltonian $H_{\text{in}} + H_{\text{prop}}$ spans the space of the Ω-circuit truth table restricted to the desired inputs, since all other input combination have received an energy penalty. The spectrum of the Hamiltonian still has a ground state energy of zero and a spectral gap to the next eigenvalue of at least δ. To mitigate this problem, one adds a small perturbation to the qubit representing the Ω-circuits output. Denote this perturbation as H_{out} and define it as $b(|0\rangle\langle 0| - |1\rangle\langle 1|)$. Now the total Hamiltonian is a sum of terms $H_{\text{in}} + H_{\text{prop}} + H_{\text{out}}$.

Completeness: It is now easy to show the existence of an eigenvalue at most a if the Ω-circuit accepts input vector $|\eta\rangle$. It then follows that $\langle\eta|H_{\text{in}}|\eta\rangle = \langle\eta|H_{\text{prop}}|\eta\rangle = 0$. It is easy to show that $\langle\eta|H_{\text{out}}|\eta\rangle \leq a$ which recovers the desired bound.

Soundness: For the case that the Ω-circuit rejects, we must show that all eigenvalues are at least b. Let us apply Lemma 14 inside the space $\mathcal{L}^{\perp}$ with $H_2 = H_{\text{prop}}$ and $H_1 = H_{\text{in}} + H_{\text{out}}$ which recovers the lower bound $\lambda(H) \geq b$. □

VI. NOVEL 3-LOCAL GADGETS

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

$$H_{\text{target}} = Y + J\sigma_1 \otimes \sigma_2 \otimes \sigma_3, \tag{35}$$

where Y is diagonal in the σ basis. We will write the spectrum of $\sigma_1 \otimes \sigma_2 \otimes \sigma_3$, in canonical (Boolean counting) order, as

$$\{1, -1, -1, 1, -1, 1, 1, -1\}. \tag{36}$$

Remark 24. *The spectrum* (36) *corresponds to the Walsh function represented by the* 8^{th} *column of the matrix* $H^{\otimes 3}$*, where* H *is the* 2×2 *Hadamard matrix. We remark that* $\{\{0, 1\}, \oplus, \wedge\}$ *is the Galois field* $\mathbb{Z}_2$.

Now the low-energy, $\lambda(\sigma_1 \otimes \sigma_2 \otimes \sigma_3) = -1$, eigenspace is given as

$$\mathcal{L} = \text{span}\{|001\rangle, |010\rangle, |100\rangle, |111\rangle\}$$

and the high-energy, $+1$, eigenspace as

$$\mathcal{L}^{\perp} = \text{span}\{|000\rangle, |011\rangle, |101\rangle, |110\rangle\}.$$

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 (35) form the product $z_\star = s_1 \cdot s_2 \cdot s_3$, where $\forall i, s_i \in \{+1, -1\}$, and so we consider the group Homomorphism $\{-1, +1, \cdot\} \mapsto \{1, 0, \oplus\}$, where $\oplus$ denotes modulo 2 sum (XOR); whence

$$z_\star = x_1 \oplus x_2 \oplus x_3, \ \forall x_1, x_2, x_3 \in \{0, 1\}^3.$$

In what follows, we will present a general framework to construct the ground state of any operator in the σ basis and apply this approach to produce a 3-local gadget requiring three mediator qubits. We will then focus our attention on optimization of this new 3-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 3-variable function $z_\star$, which acts on the Hilbert space $\mathcal{H}$. This function, $z_\star$, outputs logical 0 for any input vector in $\mathcal{L}$, and for all vectors in $\mathcal{L}^\perp$ the function outputs logical 1. We will next add a small perturbation to the output $z_\star$ — thereby breaking the low-energy degeneracy and allowing us to capture the spectrum of (35) exactly, with respect to the subspace

$$\mathcal{L} + \mathcal{L}^\perp = \mathrm{span}\{|x_1x_2x_3\rangle | \forall x_1, x_2, x_3 \in \{0, 1\}\} \subset \mathcal{H}.$$

Result 25 (Three-local gadgets with three mediator qubits)**.** From Table III we know that each XOR function requires an extra qubit, and so three mediator qubits are required to create the desired coupling. Let us write the Hamiltonian that applies the XOR penalty to the variables x_1 and x_2 as $H_\oplus(x_1, x_2, y_\star, m_1)$ and the Hamiltonian that applies the XOR penalty to the variables x_3 and $y_\star$ as $H_\oplus(x_3, y_\star, z_\star, m_2)$. Now order the variables as $|x_1x_2x_3\rangle|z_\star\rangle|y_\star m_1 m_2\rangle$, where m_1 and m_2 are mediator qubits and $y_\star$ is a temporary variable that is not read. To split the spectrum into it's respective low-energy ($\mathcal{L}$) and high-energy ($\mathcal{L}^\perp$) subspaces we add the perturbation $V = J(|0\rangle\langle 0| - |1\rangle\langle 1|)$, which acts on the qubit $z_\star$. This allows one to construct the Hamiltonian (35), with the desired spectrum since the commutator $[Y, J\sigma_1 \otimes \sigma_2 \otimes \sigma_3] = 0$ shows that Y only adds energy shifts and not level mixing — see Lemma 14.

Result 26 (Three-local gadgets with two mediator qubits)**.** Let us present an alternative approach to realizing a 3-local gadget which requires only two mediator qubits. To construct the gadget Hamiltonian, consider the 2-local coupling $z_4^\star s_3$ and add the Hamiltonian that forces a penalty whenever $z_4^\star$ is not equal to the XNOR of variables x_2 and x_3. The 2-local Hamiltonian is written as $H_\oplus(x_1, x_2, z_4^\star) + z_4^\star s_3$, where $H_\oplus$ is found in Table III, and $z_4^\star$ is a temporary variable. The Hamiltonian (37) captures the desired spectrum for $\delta > 2|J|$.

$$H = \frac{\delta}{2}(4 + \sigma_2\sigma_3 + (\sigma_2 + \sigma_3)\sigma_4 + 2(\mathbb{1} - \sigma_2 - \sigma_3 - \sigma_4)\sigma_5 - \sigma_2 - \sigma_3 - \sigma_4) + \underbrace{J\sigma_1\sigma_4}_{s_1 z_4^\star}. \tag{37}$$

The ground space of the Hamiltonian (37) is given as

$$\mathcal{L} = \text{span}\{|001\rangle|00\rangle, |010\rangle|11\rangle, |100\rangle|11\rangle, |111\rangle|01\rangle\}$$

and the first excited space as

$$\mathcal{L}^\perp = \text{span}\{|000\rangle|01\rangle, |100\rangle|00\rangle, |110\rangle|00\rangle, |110\rangle|10\rangle\},$$

where the qubits are in ascending order: qubit 4 represents the Boolean XNOR of qubits 2 and 3, while qubit 5 is the mediator qubit needed to construct the XNOR function.

We will now state then prove Theorem 27 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 2-body Hamiltonians, formally we

Theorem 27. *Let H_k be a k-local Hamiltonian diagonal in any basis σ and let this Hamiltonian act on the Hilbert space $\mathcal{H}_k$. Assert that H_k has bounded norm, and let the strictly increasing list $\{E_1, E_2, \cdots, E_k\}$ denote the eigenenergies of H_k formed by combing degeneracies, and label the corresponding eigenspaces as $\{\mathcal{L}_1, \mathcal{L}_2, \cdots, \mathcal{L}_k\}$, respectively. Then there exists a 2-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 $\{\mathcal{L}_1, \mathcal{L}_2, \cdots, \mathcal{L}_k\}$. In particular, there exists a 2-local reduction capturing the k energy subspaces $\{\mathcal{L}_1, \mathcal{L}_2, \cdots, \mathcal{L}_k\}$ in the low-energy subspace H_k.*

Proof. Let us review the general method to construct ground states. First, determine $\mathcal{L}$, the low-energy subspace, and let E_g denote the ground state energy. One will next write a function, $z_\star = f(x_1, x_2, \ldots, x_n)$, that outputs 0 for all input vectors in $\mathcal{L}$, 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 $|x_1\rangle|x_2\rangle, \ldots, |x_n\rangle$. To capture the desired ground space, a perturbation ($V = E_g|0\rangle\langle 0|$) is added, which only acts on the qubit $z_\star$. Assume that we are instead interested in capturing several energy subspaces, with energies $\{E_1, E_2, \cdots, E_k\}$, and let us label these spaces as $\{\mathcal{L}_1, \mathcal{L}_2, \cdots, \mathcal{L}_k\}$, 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 $V = \sum_{j=1}^{k} E_j|0\rangle\langle 0|_j$. □

Example 28 (Three-body gadget with a single mediator qubit: the $\sigma\sigma\sigma$-gadget)**.** Modern experimental implementations of adiabatic quantum computers typically are limited to only being able to couple spins with one type of coupling (e.g. $\sigma_z\sigma_z$). In such a case, the standard gadget Hamiltonian approach will not work as these gadgets require multiple couplers types. We will now provide a penalty Hamiltonian which avoids this problem by relying on a new type of gadget, allowing one to introduce an extra qubit, to create an effective $\sigma_z\sigma_z\sigma_z$ in a low energy subspace.

Let us first assume that we have access to a penalty function $H_{\text{AND}}(x_1, x_2, x_3)$, where $x_i \in \{0, 1\}$ such that $H_{\text{AND}} = 0$ any time $x_3 = x_1x_2$ and is greater than some large constant Δ for all $x_3 \neq x_1 \wedge x_2$. Now consider the matrix formed by the operator coupling three spins, that is $\sigma_z\sigma_z\sigma_z$. This operator provides a representation of the spin variable product $s_1s_2s_3$. Now let us consider the group homomorphism between indicator variables x_i and spin variables s_i

$$s_i = 1 - 2x_i \tag{38}$$

to map from spin variables to indicator variables we write

$$(1 - 2x_1)(1 - 2x_2)(1 - 2x_3) = 1 - 2x_1 - 2x_2 + 4x_1x_2 - 2x_3 + 4x_1x_3 + 4x_2x_3 - 8x_1x_2x_3 \tag{39}$$

$$= 1 - 2x_1 - 2x_2 + 4x_1x_2 - 2x_3 + 4x_1x_3 + 4x_2x_3 - 8z^\star x_3 + H_{\text{AND}}(x_1, x_2, z^\star), \tag{40}$$

where (40) holds in the low energy subspace. The penalty function above would complete our task provided $H_{\text{AND}}(x_1, x_2, z^\star)$ required only two-body interactions. In Section V by solving a system of constraints, such a penalty function is possible from the 2-body Hamiltonian:

$$H_{\text{AND}}(x_1, x_2, z_\star) = \Delta(3z_\star + x_1 x_2 - 2z_\star x_1 - 2z_\star x_2). \tag{41}$$

To write this Hamiltonian in terms of spin variables in a matrix representation, first change each variable, x_i, to its operator form by the replacement $x_i \to |0\rangle\langle 0|_i$. The change to spin variables is then accomplished by the replacement: $|0\rangle\langle 0|_i \to \frac{1}{2}(\mathbb{1} - \sigma_i)$. After these substitutions one arrives at the Hamiltonian (42) which is isomorphic to (41).

$$H_{\text{AND}}(-s_1, s_2, s_\star) = \frac{1}{4}(3 + \sigma_1 - \sigma_2 + 2\sigma_\star - \sigma_1\sigma_2 + 2\sigma_1\sigma_\star - 2\sigma_2\sigma_\star) \tag{42}$$

VII. OUTLOOK AND CONCLUDING REMARKS

In this study, we have exposed a compositional structure (e.g. a ground state logic) in the span of the ground space of Hamiltonians. We connected this ground state logic to modern methods in Algebra and Category Theory. We 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 through the introduction of ancillary qubits. For ease of reference, our results are summarized in Table III and Table IV. In Theorem 27 we presented a novel 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.

VIII. ACKNOWLEDGMENTS

We thank John Baez, Stephen Jordan, Peter J. Love and Barbara Terhal. Parts of this work received funding from EC FP6 STREP QICS and the Faculty of Arts and Sciences at Harvard University. JDB completed large parts of this work visiting the Center for Quantum Technologies, at the National University of Singapore (these visits were hosted by Vlatko

Vedral).

---

[1] A. Joyal and R. Street. The geometry of tensor calculus i. *Advances in Mathematics*, 88(55), 1991.

[2] Saunders Mac Lane. Categories for the working mathematician 2nd ed. *Graduate Texts in Mathematics, Springer*, 1998.

[3] Samson Abramsky and Bob Coecke. Categorical quantum mechanics. *Chapter in the Handbook of Quantum Logic and Quantum Structures vol II, Elsevier*, 2008.

[4] P. Selinger. A survey of graphical languages for monoidal categories. *ArXiv e-prints*, August 2009.

[5] Yves Lafont. Towards an algebraic theory of boolean circuits. *Journal of Pure and Applied Algebra*, 184:2003, 2003.

[6] S. Kirkpatrick et al. Optimization by simulated annealing. *Science*, 220(4598):671–680, May 1983.

[7] J. Brooke, D. Bitko, T.F. Rosenbaum, and G. Aeppli. Quantum annealing of a disordered magnet. *Science*, 284:779, 1999. `cond-mat/0105238`.

[8] E. Farhi, J. Goldstone, S. Gutmann, and M. Sipser. Quantum adiabatic evolution algorithms with different paths. *Science*, 292(5516):472–475, 2000. `quant-ph/0208135`.

[9] Roman Orus. Two slightly-entangled NP-complete problems. *Quantum Information and Computation*, 5:449, 2005. `quant-ph/0502022`.

[10] J. D. Biamonte. Nonperturbative k -body to two-body commuting conversion hamiltonians and embedding problem instances into ising spins. *Phys. Rev. A*, 77(5):052331, 2008.

[11] F. Barahona. On the computational complexity of the Ising spin glass models. *J. Phys. A: Math. Gen.*, 15:3241–3253, 1982.

[12] A. Kitaev, A. Shen, and M. Vyalyi. Classical and quantum computation. *AMS, Graduate Studies in Mathematics*, 47, 2002.

[13] R. Feynman. Quantum mechanical computers. *Optics News (now OPN)*, 11(11):11–22, February 1982.

[14] Julia Kempe and Oded Regev. 3-LOCAL HAMILTONIAN is QMA-complete. *Quantum Computation and Information*, 3(3):258–264, 2003. `quant-ph/0302079`.

$\lvert x_1x_2x_3\rangle$	$\lvert z_\star\rangle$	$\lvert y_\star\rangle$
$\lvert 000\rangle$	$\lvert 0\rangle$	$\lvert 0\rangle$
$\lvert 001\rangle$	$\lvert 1\rangle$	$\lvert 0\rangle$
$\lvert 010\rangle$	$\lvert 0\rangle$	$\lvert 0\rangle$
$\lvert 011\rangle$	$\lvert 1\rangle$	$\lvert 0\rangle$
$\lvert 100\rangle$	$\lvert 0\rangle$	$\lvert 0\rangle$
$\lvert 101\rangle$	$\lvert 1\rangle$	$\lvert 0\rangle$
$\lvert 110\rangle$	$\lvert 1\rangle$	$\lvert 1\rangle$
$\lvert 111\rangle$	$\lvert 1\rangle$	$\lvert 1\rangle$

TABLE II. Ground state truth table generated for the Hamiltonian (21). The function output, $z_\star$, is equal to $x_1 \wedge x_2 \vee x_3$. It is instructive to think of the variable $y_\star$ as a *coupler* that follows the variables x_1 and x_2 as $y_\star = x_1 \wedge x_2$.

function	2-local Hamiltonian $\mathrm{H}(x_1, x_2, z_\star) =$	ground state (ordered: $\lvert x_1\rangle\lvert x_2\rangle\lvert z_\star\rangle$)
$0 = z_\star$	$\frac{1}{2}(\mathbb{1} - \sigma_3)$	$\mathrm{span}\{\lvert x_1x_2\rangle\lvert 0\rangle \lvert \forall x_1, x_2 \in \{0,1\}\}$
$1 = z_\star$	$\frac{1}{2}(\mathbb{1} + \sigma_3)$	$\mathrm{span}\{\lvert x_1x_2\rangle\lvert 1\rangle \lvert \forall x_1, x_2 \in \{0,1\}\}$
$\bar{x}_1 \wedge \bar{x}_2 = z_\star$	$\frac{1}{4}(3 + \sigma_1 + \sigma_2 - 2\sigma_\star + \sigma_1\sigma_2 - 2\sigma_1\sigma_\star - 2\sigma_2\sigma_\star)$	$\mathrm{span}\{\lvert 001\rangle, \lvert 010\rangle, \lvert 100\rangle, \lvert 110\rangle\}$
$\bar{x}_1 \wedge x_2 = z_\star$	$\frac{1}{4}(3 + \sigma_1 - \sigma_2 + 2\sigma_\star - \sigma_1\sigma_2 + 2\sigma_1\sigma_\star - 2\sigma_2\sigma_\star)$	$\mathrm{span}\{\lvert 000\rangle, \lvert 011\rangle, \lvert 100\rangle, \lvert 110\rangle\}$
$x_1 \wedge x_2 = z_\star$	$\frac{1}{4}(3 - \sigma_1 - \sigma_2 + 2\sigma_\star + \sigma_1\sigma_2 - 2\sigma_1\sigma_\star - 2\sigma_2\sigma_\star)$	$\mathrm{span}\{\lvert 000\rangle, \lvert 010\rangle, \lvert 100\rangle, \lvert 111\rangle\}$
$x_1 \wedge \bar{x}_2 = z_\star$	$\frac{1}{4}(3 - \sigma_1 + \sigma_2 + 2\sigma_\star - \sigma_1\sigma_2 - 2\sigma_1\sigma_\star + 2\sigma_2\sigma_\star)$	$\mathrm{span}\{\lvert 000\rangle, \lvert 010\rangle, \lvert 101\rangle, \lvert 110\rangle\}$
$x_1 \vee x_2 = z_\star$	$\frac{1}{4}(4 + \sigma_1 + \sigma_2 - 2\sigma_\star + 2\sigma_1\sigma_2 - 3\sigma_1\sigma_\star - 3\sigma_2\sigma_\star)$	$\mathrm{span}\{\lvert 000\rangle, \lvert 011\rangle, \lvert 101\rangle, \lvert 111\rangle\}$
$x_1 \vee \bar{x}_2 = z_\star$	$\frac{1}{4}(4 + \sigma_1 - \sigma_2 - 2\sigma_\star - 2\sigma_1\sigma_2 - 3\sigma_1\sigma_\star + 3\sigma_2\sigma_\star)$	$\mathrm{span}\{\lvert 001\rangle, \lvert 010\rangle, \lvert 101\rangle, \lvert 111\rangle\}$
$\bar{x}_1 \vee \bar{x}_2 = z_\star$	$\frac{1}{4}(4 - \sigma_1 - \sigma_2 + 2\sigma_\star + 2\sigma_1\sigma_2 - 3\sigma_1\sigma_\star - 3\sigma_2\sigma_\star)$	$\mathrm{span}\{\lvert 001\rangle, \lvert 011\rangle, \lvert 101\rangle, \lvert 110\rangle\}$
$\bar{x}_1 \vee x_2 = z_\star$	$\frac{1}{4}(4 - \sigma_1 + \sigma_2 - 2\sigma_\star - 2\sigma_1\sigma_2 + 3\sigma_1\sigma_\star - 3\sigma_2\sigma_\star)$	$\mathrm{span}\{\lvert 001\rangle, \lvert 011\rangle, \lvert 100\rangle, \lvert 111\rangle\}$
$x_1 \not\Leftrightarrow z_\star$	$\frac{1}{2}(\mathbb{1} + \sigma_1\sigma_3)$	$\mathrm{span}\{\lvert 0x_21\rangle, \lvert 1x_20\rangle \lvert \forall x_2 \in \{0,1\}\}$
$x_2 \Leftrightarrow z_\star$	$\frac{1}{2}(\mathbb{1} - \sigma_2\sigma_3)$	$\mathrm{span}\{\lvert x_100\rangle, \lvert x_111\rangle \lvert \forall x_1 \in \{0,1\}\}$
$x_1 \Leftrightarrow z_\star$	$\frac{1}{2}(\mathbb{1} - \sigma_1\sigma_3)$	$\mathrm{span}\{\lvert 0x_20\rangle, \lvert 1x_21\rangle \lvert \forall x_2 \in \{0,1\}\}$
$x_2 \not\Leftrightarrow z_\star$	$\frac{1}{2}(\mathbb{1} + \sigma_2\sigma_3)$	$\mathrm{span}\{\lvert x_101\rangle, \lvert x_110\rangle \lvert \forall x_1 \in \{0,1\}\}$
$x_1 \oplus x_2 = z_\star$	$4 + \sigma_1\sigma_2 + (\sigma_1 + \sigma_2)\sigma_\star + 2(\mathbb{1} - \sigma_1 - \sigma_2 - \sigma_\star)\sigma_4 - \sigma_2 - \sigma_\star - \sigma_4$	$\mathrm{span}\{\lvert 0000\rangle, \lvert 0111\rangle, \lvert 1011\rangle, \lvert 1101\rangle\}$
$x_1 \odot x_2 = z_\star$	$4 - \sigma_1\sigma_2 + (\sigma_1 - \sigma_2)\sigma_\star + 2(\mathbb{1} - \sigma_1 + \sigma_2 - \sigma_\star)\sigma_4 + \sigma_2 - \sigma_\star - \sigma_4$	$\mathrm{span}\{\lvert 0100\rangle, \lvert 0011\rangle, \lvert 1111\rangle, \lvert 1001\rangle\}$

TABLE III. Logical gadgets (Section V): The span of the zero energy ground space ($\mathcal{L}$) of these gadget Hamiltonians represent the truth table of a given switching function in the spin variables (as, for instance, the AND function: $\mathcal{L} = \mathrm{span}\{\lvert x_1x_2\rangle\lvert z_\star\rangle \lvert z_\star = x_1 \wedge x_2, \forall x_1, x_2 \in \{0,1\}\}$). This table includes all $16 = 2^{2^n}$ possible boolean functions with $n = 2$ inputs.

3-local coupling	2-local Hamiltonian
$Jx_1 \wedge x_2 \wedge x_3$	$\frac{1}{4}(4 - \sigma_1 - \sigma_2 + 3\sigma_\star + \sigma_3 + \sigma_1\sigma_2 - 2\sigma_1\sigma_\star - 2\sigma_2\sigma_\star + J\sigma_\star\sigma_3)$
$J\sigma_1 \otimes \sigma_2 \otimes \sigma_3$	$\frac{\delta}{2}(4 + \sigma_2\sigma_3 + (\sigma_2 + \sigma_3)\sigma_4 + 2(\mathbb{1} - \sigma_2 - \sigma_3 - \sigma_4)\sigma_5 - \sigma_2 - \sigma_3 - \sigma_4) + J\sigma_1\sigma_4$

TABLE IV. 3-local gadgets (See also Example 28). Top (Section V): Hamiltonian with a low-energy subspace that couples three Boolean variables. The state of the mediator qubit $\sigma_\star$ is a function (the AND) of qubits 1 and 2. Bottom (Section VI): Hamiltonian with low-energy subspace that couples three spin variables for $\delta > 2|J|$. The ground space, $\mathcal{L} = \mathrm{span}\{\lvert 001\rangle\lvert 00\rangle, \lvert 010\rangle\lvert 11\rangle, \lvert 100\rangle\lvert 11\rangle, \lvert 111\rangle\lvert 01\rangle\}$ and the first excited space, $\mathcal{L}^\perp = \mathrm{span}\{\lvert 000\rangle\lvert 01\rangle, \lvert 100\rangle\lvert 00\rangle, \lvert 110\rangle\lvert 00\rangle, \lvert 110\rangle\lvert 10\rangle\}$ — the qubits are in ascending order: qubit 4 represents the Boolean XNOR of qubits 2 and 3, while qubit 5 is the mediator qubit needed to construct the XNOR function.

[15] D. Nagaj and S. Mozes. A new construction for a QMA-complete 3-LOCAL HAMILTONIAN. *Journal of Mathematical Physics*, 48:2104, 2007. `quant-ph/0612113`.

[16] J. Kempe, A. Kitaev, and O. Regev. The complexity of the LOCAL HAMILTONIAN problem. *SIAM J. Computing*, 35(5):1070–1097, 2006. `quant-ph/0406180`.

[17] R. Oliveira and B. Terhal. The complexity of quantum spin systems on a two-dimensional square lattice. 2006. `quant-ph/0504050`.

[18] Jacob D. Biamonte and Peter J. Love. Realizable hamiltonians for universal adiabatic quantum computers. *Phys. Rev. A*, 78:012352, 2008.

[19] Y. Liu, M. Christandl, and F. Verstraete. N-representability is QMA-complete. 2006. `quant-ph/0609125`.

[20] D. Aharonov, D. Gottesman, and J. Kempe. The power of quantum systems on a line. 2007. `arXiv:0705.4077`.

[21] S. Irani. The complexity of quantum systems on a one-dimensional chain. 2007. `arXiv:0705.4067`.

[22] E. Farhi, J. Goldstone, and S. Gutmann. Quantum computation by adiabatic evolution. *MIT-CTP-3297*, 2002. `quant-ph/0001106`.

[23] D. Aharonov et al. Adiabatic quantum computation is equivalent to standard quantum computation. *SIAM Journal of Computing*, 37:166–194, 2007. `quant-ph/0405098`.

[24] I. Wegener. The complexity of boolean functions. *Wiley-Teubner*, 1987. online at: `http://eccc.hpi-web.de/`.

[25] E. Boros and P.L. Hammer. Pseudo-boolean optimization. *Discrete Applied Mathematics*, 123(1-3):155–225, 2002.

[26] T. Yamamoto et al. Demonstration of conditional gate operation using superconducting charge qubits. *Nature*, 425:941–944, 2003.

[27] I. Chiorescu, Y. Nakamura, C.J.P.M. Harmans, and J.E. Mooij. Coherent quantum dynamics of a superconducting flux qubit. *Science*, 2003.

[28] R. Harris et al. Sign and magnitude tunable coupler for superconducting flux qubits. *Phys. Rev. Lett.*, 98:177001, 2007. `cond-mat/0608253`.

[29] I. J. Crosson, D. Bacon, and K. R. Brown. Making classical ground-state spin computing fault-tolerant. *Phys. Rev. E* , 82(3):031106–+, September 2010.

[30] A. Perdomo, C. Truncik, I. Tubert-Brohman, G. Rose, and A. Aspuru-Guzik. Construction of model Hamiltonians for adiabatic quantum computation and its application to finding low-energy conformations of lattice protein models. *Phys. Rev. A* , 78(1):012320–+, July 2008.

[31] M. Gu, C. Weedbrook, Á. Perales, and M. A. Nielsen. More really is different. *Physica D Nonlinear Phenomena*, 238:835–839, May 2009.

[32] Jacob Biamonte, Stephen Clark, Mark Williamson, and Vlatko Vedral. The Quantum Theory of Information and Computation. *Oxford Graduate Course*, TT2010. www.comlab.ox.ac.uk/activities/quantum/course/.

[33] C. Kassel. Quantum groups. *Springer Graduate Texts in Mathematics*, 1994.

[34] Joachim Kock. Frobenius algebras and 2-d topological quantum field theories. *Cambridge University Press*, 2003.

[35] Bob Coecke and Ross Duncan. Interacting quantum observables: Categorical algebra and diagrammatics. *aXriv preprint 0906.4725*, 2009.

[36] K. Rosen. Discrete mathematics and its applications. *McGraw-Hill*, 1999.

[37] D. Aharonov and T. Naveh. Quantum NP-a survey. 2002. quant-ph/0210077.

Appendix A: Projection Lemma

We will now prove Lemma 14 which is discussed on page 3 in Section III. Consider first the case that $\lambda(H) \leq \lambda(H_1|_{\mathcal{L}})$. Denote by $|\eta\rangle \in \mathcal{L}$ the minimizing eigenvector of $H_1|_{\mathcal{L}}$ with eigenvalue $\lambda(H_1|_{\mathcal{L}})$. Since $H_2|\eta\rangle = 0$,

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

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

$$\min_{|\zeta\rangle\in\ \mathcal{L}+\mathcal{L}^{\perp}} \{\langle\zeta|H|\zeta\rangle\} \leq \langle\eta|H|\eta\rangle = \lambda(H_1|_{\mathcal{L}}),$$

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

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

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

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

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

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

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

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

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 Section V 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 such as the wikipedia entry (`http://en.wikipedia.org`), the articles linked to therein as well as the straight forward reference [36]. This Appendix briefly introduces these maps to make the present paper self contained.

Karnaugh maps (see Fig 12 for three examples), or more compactly K-maps, are organized so that the truth table of a given equation, such as a Boolean equation ($f : \mathbb{B}^n \to \mathbb{B}$) or multi-linear form ($f : \mathbb{B}^n \to \mathbb{R}$), 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 K-map can be used to derive a minimized function.

To use a K-map to minimize a Boolean function one *covers* the 1s 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^n for any constant function $f = 1$. Fig 12 a.) and b.) contain three circles each — all of 2 and 4 boxes respectively. After the 1s are covered, a term in a *sum of products expression* [24] 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 ($\overline{x_i}$). Doing this for every covering yields a function which *matches* the truth table.

For instance consider Fig 12 a.) and b.). Here the boxes contain simply labels representing the decimal value of the corresponding Gray code ordering. The circling in Fig 12 a.) would correspond to the truth vector (ordered $z_\star, x_1$ then x_2)

$$(0, 0, 0, 1, 0, 1, 1, 1)^T . \tag{B1}$$

The cubes 3 and 7 circled in Fig 12 correspond to the sum of products term x_1x_2. Likewise (5,7) corresponds to $z_\star x_2$ and finally (7,6) corresponds to $z_\star x_1$. The sum of products representation of (B1) is simply

$$f(z_\star, x_1, x_2) = x_1x_2 \vee z_\star x_2 \vee z_\star x_1.$$

Let us repeat the same procedure for Fig 12 b.) by again assuming the circled cubes correspond to 1s in the functions truth table. In this case one finds $z_\star$ for the circling of cubes ladled (4,5,7,6), x_2 for (1,3,5,7) and x_1 for (3,2,7,6) resulting in the function

$$f(z_\star, x_1, x_2) = x_1 \vee z_\star \vee x_2.$$

Our use of K-maps in Section V allows one to visualize cube groups (variable products) that are at most 2-local in size — the highest order terms realizable with 2-local Hamiltonians. In addition, K-maps help reduce the number of simultaneous equations that, as seen in Section V, must be solved — see (31) and (41). The Karnaugh maps shown in Fig. 12 a.) and b.) illustrate groupings for quadratic and linear interactions, respectively corresponding to 2-body terms and 1-local fields. In Section V, this observation allowed us to derive 2-local Hamiltonians and prove which Hamiltonians are not possible to construct given specific numbers of mediator qubits.