Effective gaps are not effective: quasipolynomial classical simulation of obstructed stoquastic Hamiltonians

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(Dated: April 23, 2020)

All known examples confirming the possibility of an exponential separation between classical simulation algorithms and stoquastic adiabatic quantum computing (AQC) exploit symmetries that constrain adiabatic dynamics to effective, symmetric subspaces. The symmetries produce large effective eigenvalue gaps, which in turn make adiabatic computation efficient. We present a classical algorithm to efficiently sample from the effective subspace of a $k$-local stoquastic Hamiltonian $H$, without a priori knowledge of its symmetries (or near-symmetries). Our algorithm maps any $k$-local Hamiltonian to a graph $G = (V, E)$ with $|V| = O(\text{poly}(n))$ where $n$ is the number of qubits. Given the well-known result of Babai \cite{babai1985}, we exploit graph isomorphism to study the automorphisms of $G$ and arrive at an algorithm quasi-polynomial in $|V|$ for producing samples from the effective subspace eigenstates of $H$. Our results rule out exponential separations between stoquastic AQC and classical computation that arise from hidden symmetries in $k$-local Hamiltonians. Furthermore, our graph representation of $H$ is not limited to stoquastic Hamiltonians and may rule out corresponding obstructions in non-stoquastic cases, or be useful in studying additional properties of $k$-local Hamiltonians.

\textbf{Introduction.}— The power of adiabatic quantum computation (AQC) with stoquastic Hamiltonians (StoqAQC), formally introduced in \cite{aharonov2004}, remains difficult to understand. While we know AQC with general Hamiltonians is universal \cite{berry2002}, one might reasonably expect that stoquastic Hamiltonians – those that have a known representation with real, non-positive off-diagonal matrix elements – are efficiently classically simulable.

AQC interpolates over a one-parameter family of Hamiltonians $H(s)$ to produce a quantum state close to the ground state of $H(s_f)$. The computational cost of this process is usually bounded by an adiabatic theorem scaling inversely in the minimal eigenvalue gap $\gamma_{\min} = \min \gamma(H(s))$ between the two lowest eigenvalues $\gamma(H(s)) = \lambda_1(H(s)) - \lambda_0(H(s))$ of $H(s)$ \cite{benenti2006,brandao2009}. Thus, an efficient simulation algorithm must scale at least sub-exponentially with $\gamma_{\min}^{-1}$. While most researchers do not expect an exponential separation between StoqAQC and classical processes (as evidenced by i.e. \cite{aharonov2004,boixo2014,bravyi2008}), the primary techniques for simulating these Hamiltonians rely on Monte Carlo (MC) methods. When comparing AQC to MC-based algorithms, there exist a number of “obstructions” that do yield exponential separations \cite{brandao2009,brandao2010,brandao2011}.

At least in the case of diffusion MC, we can quite simply see these obstructions in their most abstract. Let $\psi$ be the ground state of a Hamiltonian $H(s)$. Now, suppose that there exists some $m$ such that $|\psi_m|^2/|\psi|^2 = \Omega(1/\text{poly}(n))$, where $n$ is the number of qubits. If there exists an efficient quantum process capable of producing the state $\psi$, it will take only $O(\text{poly}(n))$ measurements of $\psi$ in the basis $\{|i\rangle \}$ to return $m$. Alternatively, suppose one has a classical algorithm that produces samples of a random variable $X \sim \psi/|\psi|_1$, or $\Pr(X = i) = |\psi_i|^2/|\psi|^2$. We have that $|\psi_m|^2/|\psi|^2 \geq 2^{-n/2} |\psi_m|^2$. When this inequality is nearly achieved, as can be the case when $H$ has a high degree of symmetry, one requires exponentially many samples of $X$ before one expects to return $m$. (For an explicit example, see \cite[Example 0]{brandao2009}). Thus, even if one has an efficient classical process for perfectly producing samples of $X \sim \psi/|\psi|^2$, may be exponentially slower than its quantum counterpart.

Indeed, the only known examples where this inequality is nearly achieved for the ground state of $H$ rely on symmetries maintained by $H(s)$, constraining adiabatic dynamics to a polynomially-sized subspace \cite{boixo2014,boixo2018,berry2018,brandao2019,brandao2019b}. This raises a natural question: is it possible to efficiently reproduce the quantum statistics of the ground state of $H(s)$ without knowing its (near) symmetries a priori?

Here we introduce a classical algorithm that efficiently discovers and leverages symmetries. The algorithm is upper bounded in its complexity by the greater of graph isomorphism (GI) on graphs with poly$(n)$ vertices, where $n$ is the number of qubits, and poly$(S)$ where $S$ is the size of the effective subspace. Since GI is solvable in quasi-polynomial time \cite{babai1985}, our algorithm scales quasi-polynomially in $n$ whenever $S$ is quasi-polynomial in $n$. This rules out exponential separations between AQC and classical algorithms for highly symmetric $k$-local, stoquastic Hamiltonians.

\textbf{Algebraic graph theory.}— In this work, we consider two different mappings from $H$ to graphs. The first, $H \mapsto \Gamma$, takes $H$ to an exponentially-sized, undi-
directed graph $\Gamma$ with spectral properties consistent with $H$. The second, $H \mapsto G$, maps $H$ to a vertex-colored, directed graph $G = (V_G, E_G)$ which incorporates all relevant symmetries of $\Gamma$. In a sense, the latter is the compact, graph representation of $\Gamma$ in the same way that $H$ in terms of Pauli matrices is the compact representation of $H$ as a matrix. $G$ can be used to reconstruct and determine equivalent vertices of $\Gamma$ via GI. This in turn allows us to efficiently determine the effective subspace of $H$. We start by describing the construction of $\Gamma$, followed by describing the algorithm in detail, in which we treat the construction of $G$ as a black box. We then go back and lay out in detail how $G$ is constructed. Refer to Appendix A for a complete, minimal example of the full process.

**Mapping I:** $H \mapsto \Gamma$ — We consider the weighted graph representation, $\Gamma = (V_\Gamma, E_\Gamma, w_\Gamma)$, of a stoquastic Hamiltonian from [18] where $V_\Gamma = \{X_b \otimes X_{b'} \}_{b, b' \in \{0,1\}^*} \cup \{\infty\}$. (We similarly define $Y_b = \otimes_j Y_{b_j}$ and $Z_b = \otimes_j Z_{b_j}$.) We assume that we are presented with a $k$-local stoquastic Hamiltonian $H \in \mathbb{R}^{[V]^k \times [V]^k}$ where $V^* = V \setminus \{\infty\}$ specifically,

$$H = -\sum_{\|b\|_H \leq k} \alpha_b X_b - \sum_{\|b\|_H \leq k} \beta_b Y_b + \sum_{\|b\|_H \leq k} \kappa_b Z_b, \quad (1)$$

where $\|b\|_H$ is the Hamming weight of the bit string $b$ and $|b\|_H \leq k$. Let $H_X = \sum_{\|b\|_H \leq k} \alpha_b X_b$ and $H_Y = \sum_{\|b\|_H \leq k} \beta_b Y_b$. Now,

$$\langle b'\rangle (H_X + H_Y) X_b | b'\rangle = \alpha_b + i^{-|b||b'|} \beta_b \langle b'\rangle Z_b | b'\rangle = \alpha_b + i^{-|b||b'|} (-1)^{b \cdot b'} \beta_b = \alpha_b + i^{2b \cdot b'} - |b||b'| \beta_b. \quad (2)$$

We let $w(u, v) = w(v, u)$,

$$w(X_{b'}, v) = \begin{cases} \alpha_b + i^{2b \cdot b'} - |b||b'| \beta_b & \text{if } v = X_b \otimes b' \\ \sum_{\|b\|_H \leq k} (-1)^{b \cdot b'} \kappa_b & \text{if } v = \infty \end{cases} \quad (3)$$

and $E_\Gamma = \{\{u, v\} \mid w(u, v) \neq 0\}$. The eigenvectors of $H$ satisfy

$$(w(u, \infty) - \lambda_i) \phi_i(u) = \sum_{v \in V^*_\Gamma} w(u, v) \phi_i(v),$$

where $u \in V^*_\Gamma$, $\phi(\infty) = 0$, and $(\phi_i, \lambda_i)$ is the $i$th eigenvector-eigenvalue pair. In order to find symmetric subspaces of $H$, we consider identifying all vertices of $\Gamma$ that are equivalent under an edge-weight preserving automorphism $f : V_\Gamma \to V_\Gamma$ of $\Gamma$. We call the set of all such automorphisms $\text{Aut}(\Gamma)$. Now, we sum over equivalence classes $[u] = \{f(u) \mid f \in \text{Aut}(\Gamma)\}$:

$$\sum_{u' \in [u]} (w(u', \infty) - \lambda_i) \phi_i(u') = \sum_{u' \in [u]} \sum_{v \in V^*_\Gamma} w(u', v) \phi_i(v),$$

or

$$(w(u, \infty) - \lambda_i) \phi_i(u) = \sum_{v \in V^*_\Gamma} \omega_{u[v]} \phi_i(v), \quad (4)$$

where $\omega_{u[v]} = \sum_{v \in [v]} w(u, v)$.

This defines our effective Hamiltonian $H' : [V^*_\Gamma] \times [V^*_\Gamma] \to \mathbb{R}^+$ on the space of effective vertices $[V^*_\Gamma] = \{[u]\}_{u \in V^*_\Gamma}$:

$$H'([u], [v]) = \begin{cases} w(u, \infty) & \text{if } [u] = [v] \\ -\omega_{u[v]} & \text{otherwise.} \quad (5) \end{cases}$$

Note that $\omega_{v[u]} \neq \omega_{u[v]}$, but rather $\|v|\omega_{v[u]} = \|u|\omega_{u[v]}$. By Eq. (4), the right eigenvector of $H'$ corresponding to eigenvalue $\lambda_0$ is proportional to the eigenvector of $H$ corresponding to eigenvalue $\lambda_0$.

The algorithm. — Assume that we can map our Hamiltonian to a graph $\Gamma$ as described above. Our goal is to find an effective graph, $\Gamma'$ with vertex set $[V^*_\Gamma] \cup \{\infty\}$, whose ground state corresponds to that of $\Gamma$.

For clarity, we break the classical algorithm into two parts: (1) FINDEfFECTIVEVERTICES, which recursively searches $\Gamma$ to return $V'$ such that $u \in V' \iff V' \cap [u] = \{u\}$; and (2) FINDREPRESENTATIVE, which takes as input $V'$ and returns $\Gamma'$. Both routines assume the existence of an ancillary algorithm FINDREPRESENTATIVE($u, V'$) = $v \in V' \cap [u]$, whose existence we will later justify. For now, we treat it as an oracle with runtime quasi-polynomial in $n$, $O(|V'\rangle \langle QP(n)|)$, where QP($n$) matches the runtime of the best-known GI algorithm [1, 20].

Algorithm 1 Find Effective Vertices

1: function FINDEfFECTIVEVERTICES($u, V'$)
2: if $u = \emptyset$ then
3: \quad $u \leftarrow \text{RANDOM}(V^*_\Gamma)$
4: \quad Add $u$ to $V'$
5: for $v \in N(u)$ do
6: \quad if FINDREPRESENTATIVE($v, V'$) = $\emptyset$ then
7: \quad \quad Add $v$ to $V'$
8: \quad \quad $V' \leftarrow \text{FINDEfFECTIVEVERTICES($v, V'$)}$
9: return $V'$

Algorithm 1 returns a set of vertices such that each vertex is distinct and the entire routine, including the FINDREPRESENTATIVE subroutine, takes time $O\left(\Delta(\Gamma)|V'|^2 QP(n)\right)$ where $\Delta(\Gamma)$ is the maximum degree of $\Gamma$. Since $V'$ includes precisely one representative of each equivalence class in the connected component of $\Gamma$, the following routine generates the effective graph $\Gamma'$. 
The primary loop of FindEffectiveGraph (Line 4) takes time $O\left(\Delta(\Gamma)|V'|^2 \text{QP}(n)\right)$, and therefore the total time to obtain the effective graph is also $O\left(\Delta(\Gamma)|V'|^2 \text{QP}(n)\right)$.

At this point, we can obtain $H'$ and sample from its eigenstates. In particular, for $u,v \in V'$, $\Omega_{uv} = \omega_{u,v} = \sum_{n \in [v]} w(u,v_0)$. Thus, Eq. (5) is well-defined and the operator $H'$ known, even if each entire equivalence class $[u]$ is not.

We know that existing methods, such as the power iteration method, can produce the ground state $\phi'$ of $H'$ with error $\epsilon$ in time $O\left(\log(\epsilon^{-1})/\log(\lambda_1/\lambda_0)\right)$. Therefore, we can sample the ground state of the full Hamiltonian $H$ in time $O\left(\log(\epsilon^{-1})/\log(\lambda_1/\lambda_0) + \Delta(\Gamma)|V'|^2 \text{QP}(n)\right)$.

We note that we cannot simply normalize $\phi'$ and expect to obtain appropriate statistics; rather, each $u \in V' \cap [u]$ represents a sample of the class itself. Thus, we need to sample $[u]$ with probability $||[u]|\phi(u)|^2$, where $\phi$ is the appropriately normalized ground state of $H$. By Eq. (4), $H'$ has a ground state $\phi'$ that preserves relative amplitudes $\frac{\phi(u)}{\phi(v)} = \frac{\phi'(u)}{\phi'(v)}$ for all $u,v \in V'$.

Now, we use $\phi'$ and $[u]$ to sample $u \in [u] \cap V'$ with probabilities according to $\phi$,

$$\Pr([u]) = ||[u]|\phi(u)|^2 = \frac{||[u]|\phi'(u)|^2}{\sum_{v \in V'} ||[v]|\phi'(v)|^2}$$

(6)

Note that for $\omega_{[u]} \neq 0$, $\frac{||[u]|}{||[v]|} = \frac{\omega_{u,v}}{\omega_{v,v_0}}$. Therefore,

$$\sum_{v \in V'} \frac{||[v]|}{\omega_{[v]}} = \left(\sum_{v \in V'} \prod_{e \in P(u,v)} \frac{\omega_{e_1}}{\omega_{e_2}}\right)^{-1}$$

(7)

where $P(u,v) \subseteq E_G$ is any directed path connecting $u,v \in V'$. Up to a factor constant for all $u,v \in V'$, Eq. (7) determines $||[u]|$ and, thus, fully determines Eq. (6).

Repeating this process initializes a new seed in Algorithm 1 Line 3, and thus we return each member of $[u]$ with equal probability. Furthermore, the random seed guarantees that a sample from a connected set of vertices $V_C$ of $\Gamma$ is returned with probability $|V_C|/|V|$, as expected.

**Mapping II: $H$ to $G$** — Now, we will explicitly give an implementation of FindRepresentative. We begin by generalizing Crawford’s formalism of clausal theories [21] to study $\text{Aut}(\Gamma)$ and build what we abusively call a “clausal theory graph” $G$. Our goal is to define an invertible map $M$ such that $M(\Gamma) = M_0[V_T] \cup M_1[E_T] = G$. We do so by introducing gadgets, smaller graphs that allow us to separately map each $v \in V_T$ and $e \in E_T$ to specific vertex-colored, directed graphs. The union of these gadgets forms $G$. We will introduce a number of different types of vertices, where each type is assigned a unique color by $\tau : V_T \rightarrow \mathbb{R}$. Superscripts will distinguish distinct vertices that are assigned the same label. (E.g., $\ell(0), \ell(1)$.) Furthermore, for simplicity, we will abusively write $\{u,v\}$ for an undirected edge and $(u,v)$ for a directed edge. (Thus, $\{u,v\} \subset E$ can be read as $\{u,v\} \in E).$

First, we define a set of literals $L = \{Z_i \}_{i=0}^{n-1}$ and their negations $-L = \{\neg Z_i \}_{i=0}^{n-1}$, where $\bar{i} = (\delta_{i,j})_{j=0}^{n-1}$. We label each vertex $X_b \in V_T$ by a set of literals $A(X_b) \subset L \cup -L$, where $A(X_b) = \{\neg Z_i \}_{i=0}^{n-1}$. Clearly, $X_b A(X_b) X_b = -A(X_b)$. We call $A(X_b)$ an assignment. Each $X_b$ corresponds to a gadget, the vertex-colored star graph $M_0(X_b)$ with edge set $E_{M_0(X_b)} = \{\{\ell(0), A(X_b)\}_{\ell \in A(X_b)}\}$, where $\tau(\ell(0)) = 0$. Furthermore, $M_0 : V_T \rightarrow \{L(0) \cup \neg L(0)\} =: \{X_b : b \in \{0,1\}\}$ is bijective and hence invertible. Thus, $M_0^{-1}(M_0(X_b)) = X_b$.

For each edge generator $X_{ab} \in K$, we construct the graph $G_1(b)$ specified by edge set $E_{G_1(b)} = \bigcup_{b \neq 0} \{\{Z_i^0 : X_b\}, \{X_b, \neg Z_i^0\}\}$. Here, $\tau(X_b) = \alpha_b$. See Figure 1a for an example.

Each $G_1(b)$ only captures weights $\alpha_b$ corresponding to edges generated by $X_b \in K$. We still require gadgets that incorporate $\beta_b$, so that we can extract edge weights consistent with Eq. (3) from $G$. Define

$$U_b = \left\{\left\{\neg Z_i^b \right\}_{b \neq 0} \mid i \in \mathbb{Z}^0, b \neq 0 \right\}.$$

**FIG. 1:** Example gadgets: (a) corresponds to Hamiltonian entries $-X_{b0} - X_{b01}$ and (b) corresponds to $-Y_{b01}$. Circles, triangles, diamonds, and hexagons are literal, generator, weight generator, and weight generator cluster vertices, respectively.
The function uses GI-MB is true by construction, but we include 1 for completeness. Now, we define $G(u) = M_0(u) \cup M_1(E_{\Gamma})$ and can state the following theorem.

**Theorem 2.** There exists a color-preserving isomorphism $G(u) \simeq G(v)$ if and only if $u \equiv v$.

Theorem 2 is also true by construction, and explicit proof can be found in Appendix B. By exploiting the $k$-local structure of the Hamiltonian in the form of a compact $G$, we are able to reduce our problem from deciding whether $f \in \text{Aut} \Gamma$ for an exponentially-sized graph $\Gamma$ to deciding isomorphism $G(u) \simeq G(f(u))$ of polynomially-sized graphs $G(u), G(f(u))$.

Armed with this construction and the above theorems we can now explicitly give the algorithm for FindRepresentative.

**Algorithm 3** Check equivalent vertices

1. function FindRepresentative\((u,V')\)
   2. $G \leftarrow G(u)$
   3. for $v \in V'$ do
      4. $G' \leftarrow G(v)$
      5. if $G \simeq G'$ then return $v$
   6. return $\emptyset$

We note that $G(u)$ can be constructed in time $O(\text{poly}(n))$ and that color-preserving GI on bipartite, directed graphs is GI-complete [23]. Additionally, Algorithm 3—checking whether there exists an $f \in \text{Aut} \Gamma$ such that $v = f(u)$—with stoquastic $k$-local Hamiltonians is GI-complete.

To see this, for any two graphs $S, S'$, label vertices such that $V_S \cap V_{S'} = \emptyset$ and let $H = \sum_{\{i,j\} \in E_S} Z_i Z_j + \sum_{\{i,j\} \in E_{S'}} Z_i Z_j$. Then, $G \left( X_{\Theta_{V \cup V'}}^{-1} \right) \simeq G \left( X_{\Theta_{V \cup V'}}^{-1} \right)$ iff $S \simeq S'$. In the other direction, Algorithm 3 uses GI as a subroutine. The best known algorithm for GI takes time $\text{QP}(n) = 2^{O(\log(n) \times O(1))}$ [1, 20], and therefore the entire routine takes $O(\|V'\| \text{QP}(n))$.

Discussion. — Our algorithm rules out the existence of an exponential separation between classical algorithms and StoqAQC using Hamiltonians with effective subspaces $|V'|$ that scale subexponentially in $n$, a class containing all previously known $k$-local obstructions [9–11] (Note that Example 1 is not $k$-local.) However, our algorithm does not preclude (a) a quasi-polynomial speedup or (b) a speedup when $|V'| = \Theta(2^n)$.

Regarding (a), it is unclear how one might solve GI using samples from the symmetric subspace and, more fundamentally, whether GI is $\Omega(\text{QP}(n))$. Nonetheless, our only goal is to return samples of a state $\psi$ that is $\epsilon$-close to the ground state of $H$, so a graph similarity algorithm such as [24] might suffice to implement FindRepresentative. Given that measuring similarity is generally NP-hard [22], we would somehow need to exploit the structure of $G$ to provide a faster algorithm.

**Theorem 1.** The function $M : \Gamma \mapsto G$ is bijective.

Theorem 1 is true by construction, but we include proof in Appendix B for completeness. Now, we define $G(u) = M_0(u) \cup M_1(E_{\Gamma})$ and can state the following theorem.
Regarding (b), our results can be extended to near-symmetries via a straightforward application of the Davis-Kahan sin Θ theorem [26, 27]. In particular, let $H$ be a Hamiltonian with ground state density matrix $\rho$ and $H + \Delta$ a perturbed version of $H$ with ground state density matrix $\rho_\Delta$ that we actually seek to sample from. Then, $$\sqrt{1 - F(\rho, \rho_\Delta)} \leq \frac{\pi}{2} \left\| (I - \rho_\Delta) \Delta \rho \right\|_F \leq \frac{\pi}{2} \tan^2 \Phi$$ where $F(\rho, \rho_\Delta) = \|\rho \rho_\Delta\|_F^2$ is the fidelity, $\tan^2 \Phi = \frac{\|\Delta\|_F^2}{\gamma(H)\|\Delta\|_F^2}$, and $\gamma(H)$ is the eigenvalue gap of $H$. Thus, $F(\rho, \rho_\Delta) \geq 1 - \frac{\pi^2}{4} \tan^4 \Phi$.

If one has any procedure for producing a guess $\rho$, one can later check that $\|\rho - \rho_\Delta\| \leq \epsilon$ as a limited example, suppose one perturbs each $\alpha_b, \beta_b, \kappa_b$ in $H$ by at most $\delta$. Then, $\|\Delta\|_F \leq \delta \|H\|_F$. Therefore, provided that $\delta \leq \epsilon \|H\|_F$, $\tan^2 \Phi \leq \frac{\pi^2}{4}$. Hence, we can achieve arbitrary precision $\epsilon$ while perturbing each of $\alpha_b, \beta_b, \kappa_b$ by $\delta = O(\epsilon^2/\|H\|_F)$, where we have assumed $\gamma/\|H\|_F = \Omega(\text{poly}^{-1} n)$ throughout. More general approximation algorithms are left for future work.

Beyond such symmetric and approximately symmetric problems, whether all $k$-local stoquastic Hamiltonians are efficiently simulable remains an open question. We conjecture that families of Hamiltonians that lack near-symmetries typically have exponentially small gaps, suggesting that they are difficult for AQC [28]. This conjecture is largely motivated by the fact that avoiding exponentially small gaps requires pathologically smooth transitions, as explained in Appendix C. Proving this, combined with our results here, would reduce understanding the simulability of StoaQC to better understanding the significance of the gap in both classical and quantum cases.

Acknowledgements.— The authors would like to thank Andrew Glaudell and Brad Lackey for useful discussions and suggestions. J.B. was supported in part by the DOE CSGF program (award No. DE-SC0019323). M.J. was supported in part by AFRL (award No. FA8750-19-C-0044). This research was supported in part by Perimeter Institute for Theoretical Physics. Research at Perimeter Institute is supported by the Government of Canada through Industry Canada and by the Province of Ontario through the Ministry of Economic Development and Innovation. J.B. also acknowledges partial funding by the DOE BES Materials and Chemical Sciences Research for Quantum Information Science program (award No. DE-SC0019449), DOE ASCR FAR-QC (award No. DE-SC0020312), NSF PFCQC program, DOE ASCR Quantum Testbed Pathfinder program (award No. DE-SC0019040), AFOSR, ARO MURI, ARL CDQI, and NSF PFC at JQI.

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For simplicity and to avoid too much notation, we consider only Hamiltonians that can be written as these combinations. However our construction will generalize to situations with mixed terms (i.e. $XYX$), by introducing a new gadget that connects together an $X$- and $Y$-gadget. See Fig. 1b.

As previously noted, we might actually have terms like $XYY$ in our Hamiltonian. To handle such situations, we can create a new gadget by joining together an appropriate $G_i$ with another $G_{j \neq i}$ by introducing an edge connecting their respective cluster vertices.

A large spectral gap is not necessary for successful AQCG. However our construction will generalize to situations with mixed terms (i.e. $XYX$), by introducing a new gadget that connects together an $X$- and $Y$-gadget.

This corresponds to a graph $\Gamma$ where $V_\Gamma^*$ is a hypercube with all edge weights $\alpha_b = 1$. The vertex $\{\infty\}$ is connected to every vertex $v \in V_\Gamma^*$ by an edge weight $w(u, \infty) = \sum_{|b|=1}(-1)^{v \cdot b + u \cdot b}$. For our example, we consider 3 qubits and assume that $v = 010$. (See Fig. 3.)

Following the steps in the main paper we can obtain the clausal theory graph for $H_{010}$ excluding assignments, $M_1(E_G)$. As can be seen in Fig. 4, including assignments for $u, v \in \Gamma$ demonstrates $u \equiv v \iff G(u) \simeq G(v)$.

We start by calling Algorithm 1 and initialize $V'$ to the empty set. Then, we choose a random vertex $v_0 \in V_\Gamma$. Suppose that $v_0 = X_{100}$, which we then add to $V'$. Now, we recursively check each neighbor of $n \in N(X_{100})$ and if it is not equivalent to an element already in $V'$, we add it to $V'$. Suppose the first neighbor we check is $n = X_{000}$. To check equivalences, we generate $G(X_{100})$ and $G(X_{000})$ as shown in Fig. 5a and Fig. 5b, respectively. One can see that these graphs are not isomorphic, so we add $X_{000}$ to $V'$. At this point, $V' = \{X_{100}, X_{000}\}$.

Having added $X_{000}$ to $V'$, we continue the recursion and check the neighbors of $X_{000}$. Suppose the first neighbor called is $X_{000}$. (See Fig. 5c for the corresponding clausal theory graph.)

Having added $X_{000}$ to $V'$, we continue the recursion and check the neighbors of $X_{000}$. Suppose the first neighbor called is $X_{000}$. (See Fig. 5c for the corresponding clausal theory graph.) Now, we see that $G(X_{001}) \simeq G(X_{100})$, so that $X_{001} \equiv X_{100}$. Because $X_{100} \in V'$, we do not add $X_{001}$ to $V'$, and this branch of the recursion terminates and we continue checking neighbors of $X_{000}$.

Next, we check $X_{010}$, and see that it gets added to $V'$. However, the recursion terminates for all of $X_{010}$’s neighbors. Having checked all neighbors of $X_{000}$, we return to finish checking neighbors of $X_{011}$. Repeating the process, we return the effective vertex set $V' = \{X_{100}, X_{000}, X_{010}, X_{101}\}$ where, as expected, we have one representative of each equivalence class of vertices of the original graph $\Gamma$ in Fig. 3.

Once we have our effective set of vertices we proceed to calculate the weights $\Omega_{av}$ in the main loop of Algorithm 2. One can walk through this loop by hand with ease obtaining the matrix.

Figure 3: $\Gamma$ for $H_{010}$. Each vertex is labeled by a member of $X_b$. The disconnected edges connect to the boundary vertex $\infty$ and are labeled by their weights.
\[ \Omega = \begin{pmatrix} 0 & 2 & 0 & 1 \\ 2 & 0 & 1 & 0 \\ 0 & 3 & 0 & 0 \\ 3 & 0 & 0 & 0 \end{pmatrix} \]

where the rows and columns are in the same order as listed above in \( V' \). Given \( \Omega \) and \( V' \) we can calculate

\[ H' = \begin{pmatrix} -1 & -2 & 0 & -1 \\ -2 & 1 & -1 & 0 \\ 0 & -3 & 3 & 0 \\ -3 & 0 & 0 & -3 \end{pmatrix} \]

from which we can compute the ground state in the symmetric subspace, \( \phi' \). We can also compute the size of each equivalence class using Eq. (7) from the main text yielding

\[ \|X_{100}\| = \|X_{000}\| = 3 \\
\|X_{010}\| = \|X_{101}\| = 1. \]

Finding the ground state eigenvector of \( H' \) gives \( \phi' = (3 + 2\sqrt{2}, 1 + \sqrt{2}, 1, 7 + 5\sqrt{2}) \). Now, we compute the probability of sampling each equivalence class using Eq. (6). That is,

\[
\Pr(\|X_{100}\|) \approx 0.032 \quad \Pr(\|X_{000}\|) \approx 0.055 \\
\Pr(\|X_{010}\|) \approx 0.003 \quad \Pr(\|X_{101}\|) \approx 0.622.
\]

We then return a member of \( V' \) according to the above-stated probability distribution. We can easily verify that this agrees with the probability that, upon computational-basis measurements, we return a member of the corresponding equivalence class of the full Hamiltonian.

### Appendix B: Proofs

**Proof of Theorem 1.** By construction \( M : \Gamma \rightarrow G \) is unique, so we only need to show that the \( M^{-1} \) exists. First, note that \( M_0 : V_\Gamma \rightarrow M_0[V_\Gamma] \subset V_G \) is bijective and provides a unique mapping from vertices to assignments of literals. Hence, we only need to show how to derive \( w(u, v) \) from \( G \) for all \( u, v \in V_\Gamma \times V_\Gamma \).

For any \( u \in V_\Gamma \), we calculate \( w(u, \infty) \) by considering all shortest paths \( P_b \) connecting \( A(u) \) to \( C_b^{(1)} \) through \( G \). The weight

\[ w(u, \infty) = 2 \sum_{b : |P_b| \neq |b|} |\kappa_b| - \sum_b |\kappa_b|. \]

Similarly, we can consider any pair \((u, X_bu) \in V_\Gamma \times V_\Gamma \). We consider \( \mathcal{M}(u, X_bu) = (L \cup -L) \setminus (M_0(u) \cap M_0(v)) \) and construct \( S = \mathcal{M}(u, X_bu) \setminus M_1(\{u, X_bu\}) \). Let \( P_b \) be the number of shortest paths connecting \( \tau_1(A(u)) \) to \( \tau_1(A(X_bu)) \) through \( S \). Then, \( w(u, X_bu) = \alpha_b + (-1)^{|P_b|} \beta_b \) if \( G_1(b) \cup G_2(b) \subset G \) and 0 otherwise.

Hence, \( \exists! M^{-1} : \Gamma \rightarrow M \) and \( M \) is bijective. \( \square \)

The following fact allows us to add and remove edges from a graph in a way that preserves isomorphism.

**Fact 1.** For graphs \( G_1 = (V, E_1), G_2 = (V, E_2) \), if \( G_1 \cong G_2 \) with isomorphism \( f : V \rightarrow V \), then \( f \) is also an isomorphism between \( G_1'(V, E_1') \) and \( G_2' = (V, E_2') \) where for any \( E \subseteq V \times V \),

1. \( E_1' = E_1 \setminus E \) and \( E_2' = E_2 \cup f[E] \); or
2. \( E_1' = E_1 \cup E \) and \( E_2' = E_2 \setminus f[E] \).

The following lemma makes use of Fact 1 to preserve equivalences. Unlike Fact 1, we also define a consistent re-labeling of vertices for each new equivalence. Thus, we show that an isomorphism \( f' \bigr|_{\mathcal{V}_G(u)} \) such that \( M_0(u) \cup M_1(E_\Gamma) \cong M_0(f(u)) \cup M_1(E_\Gamma) \) exists if and only if there exists an automorphism \( f' : V_G \rightarrow V_G \) of \( G \).

**Lemma 1.** \( f' \bigr|_{\mathcal{V}_G(u)} \) can be extended to \( f \) an automorphism of \( G \) iff \( f' \bigr|_{\mathcal{V}_G(u)} \) is a color-preserving isomorphism \( G(u) \cong G(f(u)) \), where \( f = A^{-1} \circ f' \circ A \).

**Proof.** It is clearly the case that if \( f' \) is a color-preserving automorphism of \( G \), then \( f' \bigr|_{\mathcal{V}_G(u)} \) is an isomorphism \( G(u) \cong G(f(u)) \).

For the converse, we note that trivially, \( G(u) \cap G(f(u)) = M_1(E_\Gamma) \). Thus, \( G(u)[\mathcal{V}_G(u) \setminus A(u)] \cong G(f(u))[\mathcal{V}_G(f(u)) \setminus A(f(u))] \). We now consider \( v \in V_\Gamma \), and note that \( M_0(v) \) is already defined. We extend \( f \) by \( f(v) = A^{-1}(f'(A(v))) \). By Fact 1, \( M_0(f(v)) \cup M_1(E_\Gamma) \cong M_0(v) \cup M_1(E_\Gamma) \). Since this holds for all \( v \in V_\Gamma \) and \( f \) is bijective, we take \( G = \bigcup M_1(E \cup M_1(E_\Gamma) \cong \bigcup M_0(f(v)) \cup M_1(E_\Gamma) \) and see that \( f' \) is an automorphism of \( G \). \( \square \)
FIG. 5: Some clausal theory graphs used in the example of Appendix A. Comparing Fig. 5a to Fig. 5b shows $G(X_{100}) \not\equiv G(X_{600})$ $\iff$ $X_{100} \not\equiv X_{600}$. Comparing Fig. 5a to Fig. 5c shows $G(X_{100}) \simeq G(X_{600})$ $\iff$ $X_{100} \equiv X_{600}$.

Now, we can prove Theorem 2.

Proof of Theorem 2. Suppose $u \equiv f(u) \in V_G$. By definition, $f \in \text{Aut}(\Gamma)$. By construction, we have that $g$ is a color-preserving isomorphism $G(u) \simeq G(v)$. Now, suppose that $g \big|_{V_{G(u)}}$ is a color-preserving isomorphism $G(u) \simeq G(v)$. Then, by Lemma 1, there exists some color-preserving automorphism $g : V_G \rightarrow V_G$ of $G$. Define $f(u) = A^{-1}(g(A(u)))$. Then, by Theorem 1, $f$ is an automorphism of $\Gamma$ and, thus, $u \equiv f(u)$. □

Appendix C: Smooth Transitions

We apply the result of [18] under very weak constraints to show that families of Hamiltonians almost invariably encounter an exponentially small gap, unless they undergo very smooth phase transitions. These results are similar to but, in terms of gap-analysis, stronger than those of [29]. Here, we reference only the behavior of the ground state and show that most phase transitions, like those we expect out of adiabatic optimization, produce exponentially small gaps. The following simple theorem is sufficiently illustrative, although its statement could be improved asymptotically and easily generalized to include more than $k$-local Hamiltonians.

Theorem 3. If $H$ is a $k$-local Hamiltonian with ground state $\phi$, $\|H\| \leq 1$, and there exists a set $S_0$ such that

1. $S_0 = \{u \mid |\phi(u)| < 2^{-n^c}\}$ with absolute constant $c > 0$,

2. $\sum_{u \in S_0} |\phi(u)|^2, \sum_{u \not\in S_0} |\phi(u)|^2 = \Omega \left( \frac{1}{\text{poly}(n)} \right)$,

3. and $|S_0| = O \left( \text{poly}(n) \right)$;

then $\gamma(H) = 2^{-\Omega(n^c)}$.

Proof. Note that by [30], the weighted Cheeger constant $h$ bounds $\gamma(H)$, as $2h \geq \gamma(H)$. In particular, $h = \min_S h_S$ where $h_S$ is the weighted Cheeger ratio

$$h_S = \frac{\sum_{u \in S, v \in S} (-H_{uv}) |\phi(u)||\phi(v)|}{\min \left\{ \sum_{u \in S} |\phi(u)|^2, \sum_{u \not\in S} |\phi(u)|^2 \right\}}.$$

Now, consider $S_0$,

$$h_{S_0} \leq O \left( \frac{\max_{u \in S_0} |\phi(u)|}{\min \left\{ \sum_{u \in S_0} |\phi(u)|^2, \sum_{u \not\in S_0} |\phi(u)|^2 \right\}} \right)$$

$$= O \left( \frac{\text{poly}(n) \max_{u \in S_0} |\phi(u)|}{\min \left\{ \sum_{u \in S_0} |\phi(u)|^2, \sum_{u \not\in S_0} |\phi(u)|^2 \right\}} \right)$$

$$= O \left( \frac{\text{poly}(n)2^{-n^c}}{\min \left\{ \sum_{u \in S_0} |\phi(u)|^2, \sum_{u \not\in S_0} |\phi(u)|^2 \right\}} \right)$$

$$= 2^{-\Omega(n^c)}.$$

Since the weighted Cheeger constant $h = \min_S h_S < h_{S_0} = 2^{-\Omega(n^c)}$, $\gamma(H) = 2^{-\Omega(n^c)}$. □

Thus, if we are interpolating over a family of Hamiltonians $H(s)$ and we ever encounter a ground state $\phi$ such that (1) there exists a set $S$ where we have substantial probability of returning a sample from either $S$ or $\overline{S}$, (2) for any $u \in S$ it is unlikely that we will sample $u$ in time $O(\text{poly}(n))$, and (3) $|S|$ is small, we encounter an exponentially small gap. Since we typically interpolate over a
family of Hamiltonians $H(s)$ such that the ground state $\phi_0$ of $H(0)$ has $|\phi_0(u)|^2 = O(2^{-n/2})$ for any $u$ and end in a Hamiltonian $H(1)$ such that the ground state $\phi_1$ satisfies $\sum_{u \in S} |\phi_1(u)|^2 = \Omega(1/\text{poly}(n))$ for some small set of computational basis states $|S| = O(\text{poly}(n))$, avoiding the constraints of Theorem 3 with naive families $H(s)$ is unlikely.