



On Complexity of the Quantum Ising Model

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Received: 8 January 2015 / Accepted: 23 September 2016
Published online: 11 November 2016 – © Springer-Verlag Berlin Heidelberg 2016

Abstract: We study complexity of several problems related to the Transverse field Ising Model (TIM). First, we consider the problem of estimating the ground state energy known as the Local Hamiltonian Problem (LHP). It is shown that the LHP for TIM on degree-3 graphs is equivalent modulo polynomial reductions to the LHP for general k -local ‘stoquastic’ Hamiltonians with any constant $k \geq 2$. This result implies that estimating the ground state energy of TIM on degree-3 graphs is a complete problem for the complexity class **StoqMA**—an extension of the classical class **MA**. As a corollary, we complete the complexity classification of 2-local Hamiltonians with a fixed set of interactions proposed recently by Cubitt and Montanaro. Secondly, we study quantum annealing algorithms for finding ground states of classical spin Hamiltonians associated with hard optimization problems. We prove that the quantum annealing with TIM Hamiltonians is equivalent modulo polynomial reductions to the quantum annealing with a certain subclass of k -local stoquastic Hamiltonians. This subclass includes all Hamiltonians representable as a sum of a k -local diagonal Hamiltonian and a 2-local stoquastic Hamiltonian.

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1. Introduction and Summary of Results

Numerical simulation of quantum many-body systems is a notoriously hard problem. A particularly strong form of hardness known as **QMA-completeness** [1] has been recently established for many natural problems in this category. Among them is the problem of estimating the ground state energy for certain physically-motivated quantum models such as Hamiltonians with nearest-neighbor interactions on the two-dimensional [2] and one-dimensional [3,4] lattices, the Hubbard model [5,6], and the Heisenberg model [5,7]. In contrast, a broad class of Hamiltonians known as sign-free or *stoquastic* [8] has been identified for which certain simulation tasks become more tractable. By definition, stoquastic Hamiltonians must have real matrix elements with respect to some fixed basis and all off-diagonal matrix elements must be non-positive. Ground states of stoquastic Hamiltonians are known to have real non-negative amplitudes in the chosen basis. Thus, for many purposes, the ground state can be viewed as a classical probability distribution, which often enables efficient simulation by quantum Monte Carlo algorithms [9–12]. A notable example of a model in this category is the transverse field Ising model (TIM). It has a Hamiltonian

$$H = \sum_{1 \leq u \leq n} h_u X_u + g_u Z_u + \sum_{1 \leq u < v \leq n} g_{u,v} Z_u Z_v. \quad (1)$$

Here n denotes the number of qubits (spins), $h_u, g_u, g_{u,v}$ are real coefficients, and X_u, Z_u are the Pauli operators acting on a qubit u . Note that H is a stoquastic Hamiltonian in the standard Z -basis iff $h_u \leq 0$ for all u . This can always be achieved by conjugating H with Z_u . It is known that the ground state energy and the free energy of the TIM can be approximated with an additive error ϵ in time $\text{poly}(n, \epsilon^{-1})$ using Monte Carlo algorithms [13] in the special case when the Ising interactions are ferromagnetic, that is, $g_{u,v} \leq 0$ for all u, v . Another important special case is the TIM defined on the one-dimensional lattice with $g_u = 0$. In this case the Hamiltonian Eq. (1) is exactly solvable by the Jordan–Wigner transformation and its eigenvalues can be computed analytically [14]. The ground state and the thermal equilibrium properties of the TIM have been studied in many different contexts including quantum phase transitions [15], quantum spin glasses [16,17] and quantum annealing algorithms [18–21]. In the present paper we address two open questions related to the TIM. First, we consider the problem of estimating the ground state energy of the TIM and fully characterize its hardness in terms of the known complexity classes. Secondly, we study quantum annealing algorithms with TIM Hamiltonians and show that such algorithms can efficiently simulate a much broader class of quantum annealing algorithms associated with many important classical optimization problems.

To state our main results let us define two classes of stoquastic Hamiltonians. Let $\text{TIM}(n, J)$ be the set of all n -qubit transverse field Ising Hamiltonians defined in Eq. (1) such that the coefficients $h_u, g_u, g_{u,v}$ have magnitude at most J for all u, v . A TIM Hamiltonian is said to have interactions of degree d iff each qubit is coupled to at most d other qubits with ZZ interactions. Such Hamiltonian can be embedded into a degree- d graph such that only nearest-neighbor qubits interact.

Let $\text{StoqLH}(n, J)$ be the set of stoquastic 2-local Hamiltonians H on n qubits with the maximum interaction strength J . By definition, $H \in \text{StoqLH}(n, J)$ iff

$$H = \sum_{1 \leq u < v \leq n} H_{u,v},$$

where $H_{u,v}$ is a hermitian operator acting on the qubits u, v such that $\|H_{u,v}\| \leq J$ and all off-diagonal matrix elements of $H_{u,v}$ in the standard basis are real and non-positive. One can choose different operators $H_{u,v}$ for each pair of qubits. We shall provide a more explicit characterization of 2-local stoquastic Hamiltonians in terms of their Pauli expansion in Sect. 11, see Lemma 9.

Our first theorem asserts that any 2-local stoquastic Hamiltonian can appear as an effective low-energy theory emerging from the TIM on a degree-3 graph.

Theorem 1. *Consider any Hamiltonian $H \in \text{StoqLH}(n, J)$ and a precision parameter $\epsilon > 0$. There exist $n' \leq \text{poly}(n)$, $J' \leq \text{poly}(n, J, \epsilon^{-1})$, and a Hamiltonian $H' \in \text{TIM}(n', J')$ such that*

- (1) *The i -th smallest eigenvalues of H and H' differ at most by ϵ for all $1 \leq i \leq 2^n$.*
- (2) *One can compute H' in time $\text{poly}(n)$.*
- (3) *H' has interactions of degree 3.*

Here the maximum degree of all polynomial functions is some fixed constant that does not depend on any parameters (although we expect this constant to be quite large). The theorem has important implications for classifying complexity of the Local Hamiltonian Problem (LHP) [1, 22]. Recall that the LHP is a decision problem where one has to decide whether the ground state energy E_0 of a given Hamiltonian H acting on n qubits is sufficiently small, $E_0 \leq E_{\text{yes}}$, or sufficiently large, $E_0 \geq E_{\text{no}}$. Here $E_{\text{yes}} < E_{\text{no}}$ are some specified thresholds such that $E_{\text{no}} - E_{\text{yes}} \geq \text{poly}(n^{-1})$. The Hamiltonian must be representable as a sum of hermitian operators acting on at most k qubits each, where $k = O(1)$ is a small constant. Each k -qubit operator must have norm at most $\text{poly}(n)$. Such Hamiltonians are known as k -local. Theorem 1 implies that the LHP for 2-local stoquastic Hamiltonians has the same complexity as the LHP for TIM. Indeed, consider an instance of the LHP for some Hamiltonian $H \in \text{StoqLH}(n, J)$ where $J \leq \text{poly}(n)$. Choose a precision $\epsilon = (E_{\text{no}} - E_{\text{yes}})/3$ and let H' be the TIM Hamiltonian constructed in Theorem 1. Note that H' acts on $\text{poly}(n)$ qubits and has the interaction strength $\text{poly}(n)$. Let E'_0 be the ground state energy of H' . Then $E_0 \leq E_{\text{yes}}$ implies $E'_0 \leq E_{\text{yes}} + \epsilon \equiv E'_{\text{yes}}$ and $E_0 \geq E_{\text{no}}$ implies $E'_0 \geq E_{\text{no}} - \epsilon \equiv E'_{\text{no}}$. Since $E'_{\text{no}} - E'_{\text{yes}} = (E_{\text{no}} - E_{\text{yes}})/3 \geq \text{poly}(n^{-1})$, the LHP for a 2-local stoquastic Hamiltonian has been reduced to the LHP for TIM. The converse reduction is trivial since any TIM Hamiltonian can be made stoquastic by a local change of basis. Thus we obtain

Corollary 1. *The LHP for 2-local stoquastic Hamiltonians has the same complexity as the LHP for TIM with interactions of degree 3, modulo polynomial reductions.*

It is known that the LHPs for 2-local and k -local stoquastic Hamiltonians have the same complexity for any constant $k \geq 2$, modulo polynomial reductions [8]. Thus estimating the ground state energy of TIM on a degree-3 graph is as hard as estimating the ground state energy of a general k -local stoquastic Hamiltonian for $k = O(1)$. Furthermore, the LHP for 6-local stoquastic Hamiltonians is known to be a complete problem for the complexity class StoqMA [8, 23]. This is an extension of the classical

class **MA** where the verifier can accept quantum states as a proof. To examine the proof the verifier is allowed to apply classical reversible gates in a coherent fashion and, finally, measure some fixed qubit in the X -basis. The verifier accepts the proof if the measurement outcome is ‘+’. Let $P_{acc}(x)$ be the acceptance probability of the verifier for a given problem instance x maximized over all possible proofs. A decision problem belongs to **StoqMA** if there exists a polynomial-size verifier as above and threshold probabilities $P_{yes} \geq P_{no} + \text{poly}(n^{-1})$ such that $P_{acc}(x) \geq P_{yes}$ for any yes-instance x and $P_{acc}(x) \leq P_{no}$ for any no-instance x . Here n is the length of the problem instance x , see [23] for a formal definition. Combining these known results and Corollary 1 we obtain

Corollary 2. *The Local Hamiltonian Problem for TIM with interactions of degree 3 is complete for the complexity class StoqMA.*

Finally, Theorem 1 completes the complexity classification of 2-local Hamiltonians with a fixed set of interactions proposed recently by Cubitt and Montanaro [7]. The problem studied in [7] is defined as follows. Let \mathcal{S} be a fixed set of two-qubit hermitian operators. Consider a special case of the 2-local LHP such that Hamiltonians are required to have a form $H = \sum_a x_a V_a$, where x_a is a real coefficient and V_a is an operator from \mathcal{S} applied to some pair of qubits. For brevity, let us call the above problem \mathcal{S} -LHP. The main result of Ref. [7] is that depending on the choice of \mathcal{S} , the problem \mathcal{S} -LHP is either complete for one of the complexity classes NP, QMA, or can be solved in polynomial time on a classical computer, or can be reduced in polynomial time to the LHP for TIM. In addition, one can efficiently determine which case is realized for a given choice of \mathcal{S} . Combining this result and Corollary 2 one obtains

Corollary 3. *Let \mathcal{S} be any fixed set of two-qubit hermitian operators. Then depending on \mathcal{S} , the problem \mathcal{S} -LHP is either complete for one of the complexity classes NP, StoqMA, QMA, or can be solved in polynomial time on a classical computer.*

We also prove an analogue of Theorem 1 which gives new insights on the power of quantum annealing (QA) algorithms [18, 24] with TIM Hamiltonians which received a significant attention recently [19–21]. Recall that quantum annealing (QA) [18, 24] attempts to find a global minimum of a real-valued function $f(x_1, \dots, x_n)$ that depends on n binary variables by encoding f into a diagonal problem Hamiltonian $H_P = \sum_x f(x)|x\rangle\langle x|$ acting on n qubits. To find the ground state of H_P one chooses an adiabatic path $H(\tau) = (1 - \tau)H(0) + \tau H_P$, $0 \leq \tau \leq 1$, where $H(0)$ is some simple Hamiltonian usually chosen as the transverse magnetic field, $H(0) = -\sum_{u=1}^n X_u$. Initializing the system in the ground state of $H(0)$ and traversing the adiabatic path slowly enough one can approximately prepare the ground state of H_P . The running time of QA algorithms scales as $\text{poly}(n, \delta^{-1})$, where δ is the minimum spectral gap of $H(\tau)$, see [18, 24, 25]. We focus on the special case of QA such that the objective function $f(x_1, \dots, x_n)$ is a sum of terms that depend on at most k variables each. Here $k = O(1)$ is some small constant. This includes well-known optimization problems such as k -SAT, MAX- k -SAT and many variations thereof. We show that any quantum annealing algorithm as above can be efficiently simulated by the quantum annealing with TIM Hamiltonians. The simulation has a slowdown at most $\text{poly}(n, \delta^{-1})$.

Fix some integer $k \geq 2$. We will say that H is a $(2, k)$ -local stoquastic Hamiltonian iff H is a sum of a 2-local stoquastic Hamiltonian and a k -local diagonal Hamiltonian. Let $\text{StoqLH}^*(n, J)$ be the set of all $(2, k)$ -local stoquastic Hamiltonians on n -qubits with the maximum interaction strength J .

Theorem 2. Consider any Hamiltonian $H \in \text{StoqLH}^*(n, J)$ with a non-degenerate ground state $|g\rangle$ and a spectral gap δ . There exist $n' \leq \text{poly}(n)$, $J' \leq \text{poly}(n, J, \delta^{-1})$, a Hamiltonian $H' \in \text{TIM}(n', J')$, and an isometry $\mathcal{E} : (\mathbb{C}^2)^{\otimes n} \rightarrow (\mathbb{C}^2)^{\otimes n'}$ such that

- (1) H' has a non-degenerate ground state $|g'\rangle$ and a spectral gap at least $\delta/3$.
- (2) $\| |g'\rangle - \mathcal{E}|g\rangle \| \leq 1/100$.
- (3) The isometry \mathcal{E} maps basis vectors to basis vectors.
- (4) One can compute H' and the action of \mathcal{E} , \mathcal{E}^\dagger on any basis vector in time $\text{poly}(n)$.

Here the maximum degree of all polynomial functions depends only on the locality parameter k . We note that one can replace the constant $1/100$ in condition (2) by an arbitrary precision parameter $\eta > 0$. Then the same theorem holds with a scaling $J' \leq \text{poly}(n, J, \delta^{-1}, \eta^{-1})$. One can also impose a restriction that the Hamiltonian H' has interactions of degree-3. Then a similar theorem holds, but the isometry \mathcal{E} has slightly more complicated properties, see Sect. 12 for details.

Let us discuss implications of the theorem. Suppose $H(\tau) \in \text{StoqLH}^*(n, J)$ is an adiabatic path such that $H(1) = H_P$ is the problem Hamiltonian and $H(0) = -\sum_{u=1}^n X_u$. We assume that $H(\tau)$ has a non-degenerate ground state $|g(\tau)\rangle$ and a spectral gap at least δ for all τ . Also we assume that $J \leq \text{poly}(n)$. Since X_u can be adiabatically rotated to Z_u without closing the gap, we can modify the path such that $H(0) = -\sum_{u=1}^n Z_u$. Then the initial ground state is $|g(0)\rangle = |0^{\otimes n}\rangle$. Applying Theorem 2 to each Hamiltonian $H(\tau)$ one obtains a family of TIM Hamiltonians $H'(\tau)$ such that $H'(\tau)$ has a non-degenerate ground state $|g'(\tau)\rangle \approx \mathcal{E}|g(\tau)\rangle$, the spectral gap at least $\delta/3$, and the interaction strength at most $\text{poly}(n, \delta^{-1})$. We will show that the map $H \rightarrow H'$ is sufficiently smooth, so that the family $H'(\tau)$, $0 \leq \tau \leq 1$, defines an adiabatic path and the time it takes to traverse the paths $H(\tau)$ and $H'(\tau)$ differ at most by a factor $\text{poly}(n, \delta^{-1})$, see Sect. 12 for details. Therefore one can (approximately) prepare the final state $|g'(1)\rangle$ by initializing the system in the basis state $\mathcal{E}|0^{\otimes n}\rangle \approx |g'(0)\rangle$ and traversing the path $H'(\tau)$. Measuring every qubit of the final state $|g'(1)\rangle$ in the Z -basis one obtains a string of outcomes $x \in \{0, 1\}^{n'}$ such that $\mathcal{E}|g(1)\rangle \approx |x\rangle$. Then $|g(1)\rangle \approx \mathcal{E}^\dagger|x\rangle$, that is, the ground state of H_P can be efficiently computed from x . Thus we obtain

Corollary 4. Any quantum annealing algorithm with $(2, k)$ -local stoquastic Hamiltonians can be simulated by a quantum annealing algorithm with TIM Hamiltonians. The simulation has overhead at most $\text{poly}(n, \delta^{-1})$, where n is the number of qubits and δ is the minimum spectral gap of the adiabatic path.

In the rest of this section we informally sketch the proof of the main theorems, discuss several open problems, and outline the organization of the paper.

Sketch of the proof. The proof of Theorems 1, 2 relies on perturbative reductions [2, 22] and the Schrieffer–Wolff transformation [26–28]. At each step of the proof we work with two quantum models: a simulator Hamiltonian H_{sim} acting on some Hilbert space \mathcal{H} and a target Hamiltonian H_{target} acting on a certain subspace¹ $\mathcal{H}_- \subseteq \mathcal{H}$. We represent \mathcal{H}_- as the low-energy subspace of a suitable Hamiltonian H_0 which has a large energy gap Δ for all eigenvectors orthogonal to \mathcal{H}_- . We choose $H_{\text{sim}} = H_0 + V$, where V is a weak perturbation such that $\|V\| \ll \Delta$. We show that H_{target} can be approximated by

¹ We identify H_{target} with a Hamiltonian acting on the subspace \mathcal{H}_- using a suitable encoding.

Table 1. Perturbative reductions used in the proof of Theorem 1

TIM, degree-3 graph
TIM, general graph
Hard-core dimers, triangle-free graph
Hard-core bosons, range-2
Hard-core bosons, range-1
Hard-core bosons, range-1, controlled hopping
2-local stoquastic Hamiltonians

Each model is obtained as an effective low-energy Hamiltonian for the model located one row above. The hard-core bosons (HCB) model describes a multi-particle quantum walk on a graph. The Hamiltonian consists of a hopping term, on-site chemical potential, and arbitrary two-particle interactions. Different particles must be separated from each other by a certain minimum distance that we call a range of the model. HCB is closely related to the Bose–Hubbard model. The hard-core dimers model is analogous to HCB except that admissible particle configuration must consist of nearest-neighbor pairs of particles that we call dimers. Different dimers must be separated from each other by a certain minimum distance. A rigorous definition of the models is given in Sect. 2

an effective low-energy Hamiltonian H_{eff} acting on \mathcal{H}_- which is obtained from H_{sim} using a few lowest orders of the perturbation theory,

$$H_{\text{eff}} = V_{--} - V_{-+}H_0^{-1}V_{+-} + V_{-+}H_0^{-1}V_{++}H_0^{-1}V_{+-} + \dots$$

Here V is considered as a 2×2 block matrix with the blocks labeled by ‘-’ and ‘+’ corresponding to the low-energy subspace \mathcal{H}_- and the high-energy subspace $\mathcal{H}_+ \equiv \mathcal{H}_\perp$. More precisely, $H_{\text{eff}} \approx P_- U (H_0 + V) U^\dagger P_-$, where P_- is the projector onto \mathcal{H}_- and U is a unitary operator on \mathcal{H} known as the Schrieffer–Wolff transformation, see Sect. 4. The latter brings $H_0 + V$ into a block-diagonal form such that $U(H_0 + V)U^\dagger$ preserves the subspace \mathcal{H}_- . We show that the low-lying eigenvalues and eigenvectors of H_{sim} approximate the respective eigenvalues and eigenvectors of H_{target} with an error that can be made arbitrarily small by choosing large enough Δ .

We apply the above step recursively several times such that the target Hamiltonian at the t -th step becomes the simulator Hamiltonian at the $(t + 1)$ -th step. The recursion starts from the TIM with interactions of degree-3 at the highest energy scale, goes through several intermediate models listed in Table 1, and arrives at a given 2-local or $(2, k)$ -stoquastic Hamiltonian at the lowest energy scale. Overall, the proof requires nine different reductions.²

To simplify the analysis of recursive reductions we introduce a general definition of a simulation that quantifies how close are two different models in terms of their low-lying eigenvalues and eigenvectors. Our definition is shown to be stable under the composition of simulations.

Let us informally sketch a reduction from TIM to hard-core dimer models. This reduction provides an intuitive picture of how local stoquastic interactions can be generated perturbatively by a global transverse field and allows us to highlight the role of other models from Table 1. We shall identify basis states of n qubits with configurations of particles distributed over nodes (vertices) of some graph of size n . Each node can be either empty (state 0) or occupied (state 1). Let $n_u = 0, 1$ be the occupation number of a node u and $W_{u,v}$ be the hopping operator $|10\rangle\langle 01| + |01\rangle\langle 10|$ applied to nodes u, v . The Hilbert space of the hard-core dimers (HCD) model is spanned by m -dimer

² Some of our reductions are ‘trivial’ in the sense that they simply restrict a Hamiltonian to a certain subspace. The proof contains only six ‘non-trivial’ reductions that actually change the Hamiltonian.

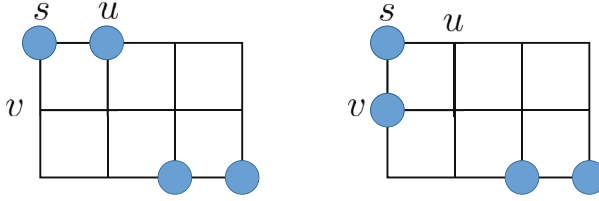


Fig. 1. Examples of 2-dimer states on the square grid. Hopping operator $W_{u,v}$ maps a 2-dimer state to another 2-dimer state

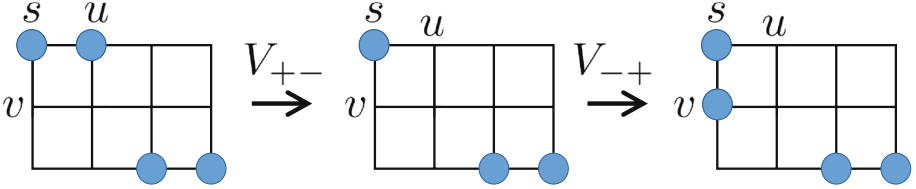


Fig. 2. Hopping term $W_{u,v}$ generated perturbatively by a global transverse field $V \sim \sum_{i=1}^n X_i$

states—configurations of $2m$ particles that consist of m well-separated particle pairs, or dimers. Each dimer must occupy an adjacent pair of nodes. For technical reasons, we require different dimers to be separated by at least three graph edges. Examples of 2-dimer states are shown on Fig. 1.

The HCD model has a Hamiltonian

$$H = H_{diag} - \sum_{1 \leq u < v \leq n} W_{u,v},$$

where H_{diag} includes only diagonal terms n_u and n_{unv} . It is understood that H is projected onto the subspace spanned by m -dimer states. Although H includes hopping terms $W_{u,v}$ between any pair of nodes, only local (next-to-nearest neighbor) hopping terms may have a non-zero projection onto the m -dimer subspace, see Fig. 1. We shall represent H as an effective low-energy Hamiltonian emerging from a TIM simulator $H_{sim} = H_0 + V$ acting on n qubits, where H_0 is a diagonal Hamiltonian chosen such that its low-energy subspace \mathcal{H}_- is spanned by m -dimers. Such Hamiltonian can be composed from terms n_u and n_{unv} , see Sect. 6. We choose the perturbation as $V = H_{diag} + h \sum_{u=1}^n X_u$. Then the first-order effective Hamiltonian is $H_{eff,1} = V_{--} = H_{diag}$ since X_u maps any dimer state to a non-dimer state which implies $P_- X_u P_- = 0$. Consider now the second-order effective Hamiltonian $H_{eff,2} = -V_{-+} H_0^{-1} V_{+-}$. The term V_{+-} can map a dimer $\{s, u\}$ to a single particle, say $\{s\}$, by annihilating the particle at u . In order to return to the m -dimer subspace, V_{-+} has to create a particle at some node v which is a nearest-neighbor of s , see Fig. 2.

Thus $H_{eff,2}$ maps a dimer $\{s, u\}$ to a dimer $\{s, v\}$ which is equivalent to applying the hopping operator $W_{u,v}$. Note that the intermediate state created by V_{+-} “remembers” location of the dimer $\{s, u\}$ since one half of the dimer is still present in the intermediate state. This is why a local hopping of dimers can emerge from the global transverse field and this is the main reason why the chain of reductions in Table 1 starts from dimers (rather than single particles hopping on a graph). We note that $H_{eff,2}$ also contains some unwanted diagonal terms. For example, an unwanted two-particle interaction $n_s n_u$ would be generated in the above example if V_{-+} creates a particle at u rather than at v . Such

unwanted terms can be easily cancelled by properly modifying V since our simulator Hamiltonian (TIM) can include two-particle interactions like $n_s n_u$. The main technical difficulty in this and other reductions is ensuring that H_{eff} does not include unwanted interactions among three or more particles such as $n_s n_u n_t$ (such terms cannot be canceled within the class TIM). For example, suppose V_{+-} creates a particle at some node i which does not belong to any dimer. In order to return to the m -dimer subspace, V_{-+} has to annihilate the particle at i . Such a process is capable of generating multi-particle interactions through the intermediate state acted upon by H_0^{-1} . To avoid this problem, we modify H_0 such that configurations with $2m + 1$ particles have much higher energy than those with $2m - 1$ particles. This ensures that V_{+-} can only annihilate particles.

Hard-core bosons (HCB) models from Table 1 describe particles hopping along edges of a graph such that the total number of particles is fixed. Loosely speaking, each particle of the HCB model is simulated by one dimer within the HCD model. Since the dimers can only move locally, it should not be too surprising that HCD allows us to simulate local hopping of particles on an arbitrary graph. HCB Hamiltonians may also contain diagonal terms n_u and $n_u n_v$. In order to avoid multi-particle interactions generated perturbatively, we have to consider several variations of HCB that differ by a *range*—the minimum distance two particles can approach each other. Our reductions only use HCB models with range $r = 1$ and $r = 2$. We also need an “enhanced” HCB model that includes controlled hopping terms such as $n_s W_{u,v}$.

To construct an HCB-simulator for a 2-local stoquastic Hamiltonian we use the dual-rail encoding of each qubit such that logical states $|0\rangle$ and $|1\rangle$ are encoded by HCB states $|10\rangle$ and $|01\rangle$ respectively. We construct simple gadgets that allow us to simulate elementary stoquastic interactions such as

$$-X \otimes |0\rangle\langle 0|, \quad -X \otimes |1\rangle\langle 1|, \quad -X \otimes X \pm Y \otimes Y$$

by HCB Hamiltonians. For example, $-X \otimes |0\rangle\langle 0|$ has an HCB-simulator $-W_{1,2} \otimes n_3$, where particles $\{1, 2\}$ encode the first qubit and particles $\{3, 4\}$ encode the second qubit. We then show how to decompose any 2-local stoquastic Hamiltonian into the elementary interactions and combine the corresponding gadgets into a single HCB simulator. The main technical difficulty here is avoiding “cross-talk” between different gadgets.

For almost all of our reductions the Hamiltonian H_0 is diagonal in the standard basis, so that all eigenvalues and eigenvectors of H_0 can be easily computed. The only exception is the reduction from TIM with interactions of degree-3 to a general TIM. For this reduction we encode each qubit of the target model into the approximately two-fold degenerate ground subspace of the one-dimensional TIM on a chain of a suitable length. Accordingly, the Hamiltonian H_0 describes a collection of one-dimensional TIMs. We simulate the logical Ising interaction $Z_u Z_v$ between some pair of logical qubits u, v by applying the physical interaction $Z_i Z_j$ to a properly chosen pair of qubits $i \in L_u$ and $j \in L_v$, where L_u is the chain encoding a logical qubit u . The logical transverse field X_u is automatically generated due to the energy splitting between the ground states of L_u . The analysis of this reduction exploits recent exact results on the form-factors of the one-dimensional TIM [29].

We emphasize that the word “reduction” is used in two distinct senses. In the present paper we speak of a perturbative reduction *from* a Hamiltonian H_{sim} *to* a Hamiltonian H_{target} when H_{target} is the effective low-energy Hamiltonian derived from H_{sim} , following terminology in physics. However, if H_{target} belongs to some particular class of Hamiltonians \mathcal{T} and H_{sim} belongs to some subclass $\mathcal{S} \subseteq \mathcal{T}$, this is a reduction *from* the class \mathcal{T} *to* the class \mathcal{S} , according to terminology in computer science.

Open problems. Our work raises several questions. First, we expect that Theorems 1 and 2 can be extended in a number of ways. For example, one may ask whether the analogue of Theorem 1 holds for TIM Hamiltonians restricted to particular families of graphs, such as planar graphs or regular lattices. We note that a simple modification of our degree reduction method based on the one-dimensional TIM produces a simulator Hamiltonian that can be embedded into the 3D lattice of dimensions $n \times n \times 2$ with periodic boundary conditions. We expect that applying additional perturbative reductions such as those described in Ref. [2] can further simplify the lattice. Likewise, we expect that Theorem 2 can be extended to the case when H is a general k -local stoquastic Hamiltonian by applying perturbative reductions of Ref. [8].

A challenging open question is whether TIM Hamiltonians defined on a 2D lattice can realize the topological quantum order. It has been recently shown that the hard-core bosons model defined on the kagome lattice has a topologically ordered ground state for a certain range of parameters [30,31]. A preliminary analysis shows that the chain of reductions from TIM to hard-core bosons described in the present paper can be modified such that all intermediate Hamiltonians have geometrically local interactions. Assuming that the unphysical polynomial scaling of interactions in the simulator Hamiltonian can be avoided [27,32], this points towards existence of topologically ordered phases described by TIM Hamiltonians.

Finally, a big open question is whether QA algorithms with TIM Hamiltonians can be efficiently simulated classically. It has been recently shown that the general purpose quantum Monte Carlo algorithms fail to simulate certain instances of the QA with TIM efficiently [33], even though these instances have a non-negligible minimum spectral gap. This leaves a possibility that some more specialized algorithms taking advantage of the special structure of TIM Hamiltonians can succeed even though the general purpose algorithm fails. Our results demonstrate that this is unlikely, since simulating the QA with TIM is as hard as simulating the QA with much more general $(2, k)$ -local stoquastic Hamiltonians.

The paper is organized as follows. Section 2 contains a rigorous definition of the models listed in Table 1. Our main technical tools are introduced in Sects. 3 and 4 which present a general definition of a simulation, describe perturbative reductions based on the Schrieffer–Wolff transformation, and prove several technical lemmas used in the rest of the paper. Section 5 shows how to simulate a general TIM Hamiltonian using a special case of TIM with interactions of degree-3. Sections 6–11 describe a chain of perturbative reductions between the models listed in Table 1. These reductions are combined together in Sect. 12, which contains the proof of Theorems 1 and 2. Finally, Appendix A proves certain bounds on eigenvalues and form-factors of the one-dimensional TIM, which are used in Sect. 5.

2. Hard-core Bosons and Dimers

Consider a graph $G = (U, E)$ with a set of n nodes U and a set of edges E . Define a Hilbert space $\mathcal{B} \cong (\mathbb{C}^2)^{\otimes n}$ with an orthonormal basis $\{|S\rangle : S \subseteq U\}$ such that basis vectors are labeled by subsets of nodes S . We shall identify subsets of nodes with configurations of particles that live at nodes of the graph. Each node can be either empty or occupied by a single particle. For any node $u \in U$ define a particle number operator n_u such that $n_u|S\rangle = |S\rangle$ if $u \in S$ and $n_u|S\rangle = 0$ otherwise. We shall often consider diagonal Hamiltonians of the following form:

$$H_{\text{diag}} = \sum_{u \in U} \mu_u n_u + \sum_{\{u,v\} \subseteq U} \omega_{u,v} n_u n_v. \quad (2)$$

Here the second sum runs over all two-node subsets (not only nearest neighbors). The coefficients μ_u and $\omega_{u,v}$ can be viewed as a chemical potential and a two-particle interaction potential respectively.

Let us now define a hopping operator $W_{u,v}$. Here $u, v \in U$ are arbitrary nodes such that $u \neq v$. By definition, $W_{u,v}$ annihilates any state $|S\rangle$ in which both nodes u, v are occupied or both nodes are empty. If one of the nodes u, v is occupied and the other node is empty, $W_{u,v}$ transfers a particle from u to v or vice versa. Matrix elements of $W_{u,v}$ in the chosen basis are

$$\langle S' | W_{u,v} | S \rangle = \begin{cases} 1 & \text{if } u \in S, v \notin S, \text{ and } S' = (S \setminus u) \cup v. \\ 1 & \text{if } v \in S, u \notin S, \text{ and } S' = (S \setminus v) \cup u, \\ 0 & \text{otherwise.} \end{cases} \quad (3)$$

Let $m, r \geq 1$ be fixed integers. Define a subspace $\mathcal{B}_m \subset \mathcal{B}$ spanned by all subsets $S \subseteq U$ with exactly m nodes. We shall refer to \mathcal{B}_m as an m -particle sector. Obviously, the operators $W_{u,v}$ and n_u preserve \mathcal{B}_m . A subset of nodes S is said to be r -sparse iff the graph distance between any distinct pair of nodes $u, v \in S$ is at least r . Define a subspace $\mathcal{B}_{m,r} \subseteq \mathcal{B}_m$ spanned by all r -sparse subsets $S \subseteq U$ with exactly m nodes. By definition, any subset of nodes is 1-sparse, so that $\mathcal{B}_{m,1} = \mathcal{B}_m$. Note that the operators $W_{u,v}$ generally do not preserve $\mathcal{B}_{m,r}$. Below we consider hopping operators $W_{u,v}$ projected onto the subspace $\mathcal{B}_{m,r}$. Matrix elements of a projected hopping operator are defined by Eq. (3), where S and S' run over all r -sparse subsets of m nodes.

Our first model is called *hard-core bosons* (HCB). It is defined on the Hilbert space $\mathcal{B}_{m,r}$, where m and r are fixed parameters. We shall refer to r as the *range* of the model. The Hamiltonian is

$$H = - \sum_{(u,v) \in E} t_{u,v} W_{u,v} + H_{\text{diag}}. \quad (4)$$

Here H_{diag} is defined by Eq. (2) and all operators are projected onto the subspace $\mathcal{B}_{m,r}$. Thus $W_{u,v}$ moves a particle only if this does not violate the r -sparsity condition. Otherwise $W_{u,v}$ annihilates a state. The coefficients $t_{u,v}$ are hopping amplitudes. We shall always assume that

$$t_{u,v} \geq 0$$

for all u, v . The coefficients μ_u and $\omega_{u,v}$ in H_{diag} may have arbitrary signs. Note that H is a stoquastic Hamiltonian. Let $\text{HCB}_r(n, m, J)$ be the set of Hamiltonians describing the m -particle sector of range- r hard-core bosons on a graph with n nodes such that all the coefficients $\mu_u, \omega_{u,v}, t_{u,v}$ have magnitude at most J . Here the Hamiltonian can be defined on any graph with n nodes. Our proof will only use HCB models with the range $r = 1, 2$. Later on we shall define certain enhanced versions of the HCB which have multi-particle interactions, see Sect. 8, and/or controlled hopping terms, see Sect. 10. We note that the HCB model with non-positive hopping amplitudes $t_{u,v} \leq 0$ has been recently studied by Childs, Gosset, and Webb [6] who showed that the corresponding LHP is QMA-complete.

Our second model is called *hard-core dimers*. This model also depends on a graph $G = (U, E)$. We shall only consider triangle-free graphs G . Let $m \geq 1$ be a fixed integer

Table 2. Classes of Hamiltonians used in the proof of Theorem 1

TIM(n, J)	Transverse field Ising Model
HCD(n, m, J)	m -dimer sector of Hard-Core Dimers model
HCB _{r} (n, m, J)	m -particle sector of Hard-Core Bosons with range r
HCB(n, m, J)	Same as HCB ₁ (n, m, J)
HCB* (n, m, J)	HCB(n, m, J) with controlled hopping terms
StoqLH(n, J)	Stoquastic 2-Local Hamiltonians

Here J denotes the maximum interaction strength and n denotes the number of nodes in the graph (the number of qubits). For those models that depend on a graph, the corresponding class is defined by taking the union over all graphs with a fixed number of nodes n (all triangle-free graphs in the case of HCD). The class HCB* is formally defined in Sect. 10

parameter. A subset of nodes $S \subseteq U$ is said to be a *dimer* iff $S = \{u, v\}$ for some pair of nodes $u \neq v$ such that $(u, v) \in E$. Define an m -*dimer* as a subset of nodes $S \subseteq U$ that can be represented as a disjoint union of m dimers S_1, \dots, S_m such that the graph distance between S_i and S_j is at least three for all $i \neq j$. This particular choice of the distance guarantees that m -dimers can be represented as ground states of a suitable Ising Hamiltonian provided that the graph is triangle-free, see Lemma 8 in Sect. 6.

Let $\mathcal{D}_m \subseteq \mathcal{B}_{2m}$ be the subspace spanned by all basis vectors $|S\rangle$ such that $S \subseteq U$ is an m -dimer. Note that the operators $W_{u,v}$ generally do not preserve \mathcal{D}_m . Below we consider hopping operators $W_{u,v}$ projected onto the subspace \mathcal{D}_m . Matrix elements of a projected hopping operator are defined by Eq. (3), where S and S' run over all m -dimers. The hard-core dimers (HCD) model has a Hilbert space \mathcal{D}_m and a Hamiltonian

$$H = -t \sum_{\{u,v\} \subseteq U} W_{u,v} + H_{\text{diag}} \quad (5)$$

where H_{diag} is defined by Eq. (2) and all operators are projected onto the subspace \mathcal{D}_m . The sum in Eq. (5) runs over all pairs of nodes (not only nearest neighbors). Although the Hamiltonian does not explicitly depend on the graph structure, the underlying Hilbert space \mathcal{D}_m does depend on the graph since the latter determines which subsets of nodes are m -dimers. A hopping process induced by $W_{u,v}$ can change a dimer $\{s, u\}$ to some other dimer $\{s, v\}$ with $u \neq v$, see Fig. 1. The coefficient t is a hopping amplitude. We shall assume that $t \geq 0$. Then H is a stoquastic Hamiltonian. Let HCD(n, m, J) be the set of Hamiltonians describing the m -dimer sector of hard-core dimers model on a graph with n nodes such that all coefficients in H have magnitude at most J . Here the Hamiltonian can be defined on any triangle-free graph with n nodes.

Some perturbative reductions described below will alter the underlying graph G . Whenever the choice of G is not clear from the context, we shall use more detailed notations $\mathcal{B}_m(G)$, $\mathcal{B}_{m,r}(G)$, and $\mathcal{D}_m(G)$ instead of \mathcal{B}_m , $\mathcal{B}_{m,r}$, and \mathcal{D}_m . Our notations for various classes of Hamiltonians are summarized in Table 2.

Finally, substituting $Z_u = I - 2n_u$ into Eq. (1) one gets

$$H = \sum_{u \in U} \mu_u n_u + \sum_{\{u,v\} \subseteq U} \omega_{u,v} n_u n_v + h_u X_u = H_{\text{diag}} + \sum_{u \in U} h_u X_u, \quad (6)$$

where $U \equiv \{1, \dots, n\}$, $\omega_{u,v} = 4g_{u,v}$ and $\mu_u = -2g_u - 2 \sum_{v \neq u} g_{u,v}$. Here we ignore the overall energy shift. Clearly, the coefficients $\omega_{u,v}$ and μ_u have magnitude at most $O(nJ)$. Below we shall work with TIM Hamiltonians as defined in Eq. (6).

3. Simulation of Eigenvalues and Eigenvectors

In this section we give a formal definition of a simulation. It quantifies how close are two different models in terms of their low-energy properties such as the low-lying eigenvalues and eigenvectors. We consider a *target* model described by a Hamiltonian H acting on some N -dimensional Hilbert space \mathcal{H} and a *simulator* model described by a Hamiltonian H_{sim} acting on some Hilbert space \mathcal{H}_{sim} of dimension at least N . Our definition of a simulation depends on a particular *encoding transformation* $\mathcal{E} : \mathcal{H} \rightarrow \mathcal{H}_{\text{sim}}$ that embeds \mathcal{H} into some N -dimensional subspace of \mathcal{H}_{sim} . We assume that \mathcal{E} is an isometry, that is, $\mathcal{E}^\dagger \mathcal{E} = I$. The encoding enables a comparison between eigenvectors of the two models. We envision a situation when the spectrum of H_{sim} consists of two well-separated groups of eigenvalues such that the N smallest eigenvalues of H_{sim} are separated from the rest of its spectrum by a large gap. Let $\mathcal{L}_N(H_{\text{sim}}) \subseteq \mathcal{H}_{\text{sim}}$ be the *low-energy subspace* spanned by the eigenvectors of H_{sim} associated with its N smallest eigenvalues.

Definition 1. Let H be a Hamiltonian acting on a Hilbert space \mathcal{H} of dimension N . A Hamiltonian H_{sim} and an isometry (encoding) $\mathcal{E} : \mathcal{H} \rightarrow \mathcal{H}_{\text{sim}}$ are said to simulate H with an error (η, ϵ) if there exists an isometry $\tilde{\mathcal{E}} : \mathcal{H} \rightarrow \mathcal{H}_{\text{sim}}$ such that

- S1. The image of $\tilde{\mathcal{E}}$ coincides with the low-energy subspace $\mathcal{L}_N(H_{\text{sim}})$.
- S2. $\|H - \tilde{\mathcal{E}}^\dagger H_{\text{sim}} \tilde{\mathcal{E}}\| \leq \epsilon$.
- S3. $\|\mathcal{E} - \tilde{\mathcal{E}}\| \leq \eta$.

For example, suppose $\mathcal{H} = \mathbb{C}^2$ and $\mathcal{H}_{\text{sim}} = \mathbb{C}^2 \otimes \mathbb{C}^2$. Consider a target Hamiltonian $H = X$ and a simulator $H_{\text{sim}} = X \otimes X + \Delta(Z \otimes Z + I)$, where $\Delta \gg 1$. Assuming that $N = 2$, the low-energy subspace of H_{sim} is spanned by $|01\rangle$ and $|10\rangle$. Consider a dual-rail encoding of a qubit, $\mathcal{E}|0\rangle = |10\rangle$ and $\mathcal{E}|1\rangle = |01\rangle$. Then $(H_{\text{sim}}, \mathcal{E})$ simulates H with an error $(0, 0)$. Indeed, choosing $\tilde{\mathcal{E}} = \mathcal{E}$ one gets $H = \mathcal{E}^\dagger H_{\text{sim}} \mathcal{E}$.

Although we do not impose any restrictions on the encoding, in practice it must be sufficiently simple. For all our reductions (except for the one of Sect. 5) the encoding \mathcal{E} maps basis vectors to basis vectors. Whenever the choice of \mathcal{E} is clear from the context, we shall just say that H_{sim} simulates H with an error (η, ϵ) . If one is interested only in reproducing eigenvalues of the target Hamiltonian, the encoding and condition (S3) can be ignored.

In the case of a zero error, $\epsilon = \eta = 0$, the target Hamiltonian H coincides with the restriction of H_{sim} onto the low-energy subspace of H_{sim} , up to a change of basis described by \mathcal{E} . Clearly, any Hamiltonian simulates itself with a zero error since one can choose $\mathcal{E} = \tilde{\mathcal{E}} = I$. We shall always assume that $\epsilon \leq \|H\|$ since otherwise the definition is meaningless (one can choose $H_{\text{sim}} = 0$ regardless of H). Note that ϵ has the dimension of energy while η is dimensionless. Loosely speaking, ϵ and η quantify simulation error for eigenvalues and eigenvectors respectively. Let us establish some basic properties of simulations.

Lemma 1 (Eigenvalue simulation). *Suppose $(H_{\text{sim}}, \mathcal{E})$ simulates H with an error (η, ϵ) . Then the i -th smallest eigenvalues of H_{sim} and H differ at most by ϵ for all $1 \leq i \leq N$.*

Proof. Property (S1) implies that the spectrum of $\tilde{\mathcal{E}}^\dagger H_{\text{sim}} \tilde{\mathcal{E}}$ coincides with N smallest eigenvalues of H_{sim} . The lemma now follows from (S2) and the standard Weyl's inequality. \square

Lemma 2 (Ground state simulation). *Suppose H has a non-degenerate ground state $|g\rangle$ separated from excited states by a spectral gap δ . Suppose $(H_{\text{sim}}, \mathcal{E})$ simulates H with an error (η, ϵ) such that $2\epsilon < \delta$. Then H_{sim} has a non-degenerate ground state $|g_{\text{sim}}\rangle$ and*

$$\|\mathcal{E}|g\rangle - |g_{\text{sim}}\rangle\| \leq \eta + O(\delta^{-1}\epsilon). \quad (7)$$

Proof. Let $|g_{\text{sim}}\rangle$ be the ground state of H_{sim} . Note that $|g_{\text{sim}}\rangle$ is non-degenerate due to Lemma 1 and the assumption $2\epsilon < \delta$. Consider an unperturbed Hamiltonian H and a perturbation $V = \tilde{\mathcal{E}}^\dagger H_{\text{sim}} \tilde{\mathcal{E}} - H$. The perturbed Hamiltonian $H + V = \tilde{\mathcal{E}}^\dagger H_{\text{sim}} \tilde{\mathcal{E}}$ has a non-degenerate ground state $\tilde{\mathcal{E}}^\dagger |g_{\text{sim}}\rangle$. Using the first-order perturbation theory for eigenvectors one gets $\| |g\rangle - \tilde{\mathcal{E}}^\dagger |g_{\text{sim}}\rangle \| \leq O(\delta^{-1}\epsilon)$ and thus $\| \tilde{\mathcal{E}} |g\rangle - |g_{\text{sim}}\rangle \| = \| \tilde{\mathcal{E}} |g\rangle - \tilde{\mathcal{E}} \tilde{\mathcal{E}}^\dagger |g_{\text{sim}}\rangle \| \leq O(\delta^{-1}\epsilon)$. Here we used the fact that $\tilde{\mathcal{E}}$ is an isometry and $|g_{\text{sim}}\rangle \in \mathcal{L}_N(H_{\text{sim}}) = \text{Im}(\tilde{\mathcal{E}})$. Property (S3) then leads to Eq. (7). \square

Importantly, our definition of a simulation is stable under compositions: if one is given some Hamiltonians H, H_1, H_2 such that H_1 simulates H with a small error and H_2 simulates H_1 with a small error, this implies that H_2 simulates H with a small error.

Lemma 3 (Composition). *Suppose (H_1, \mathcal{E}_1) simulates H with an error (η_1, ϵ_1) and (H_2, \mathcal{E}_2) simulates H_1 with an error (η_2, ϵ_2) . Let Δ_1 be the spectral gap separating N smallest eigenvalues of H_1 from the rest of the spectrum. Suppose $2\epsilon_2 < \Delta_1$ and $\epsilon_1, \epsilon_2 \leq \|H\|$. Then $(H_2, \mathcal{E}_2 \mathcal{E}_1)$ simulates H with an error (η, ϵ) , where*

$$\eta = \eta_1 + \eta_2 + O(\epsilon_2 \Delta_1^{-1}) \quad \text{and} \quad \epsilon = \epsilon_1 + \epsilon_2 + O(\epsilon_2 \Delta_1^{-1} \|H\|). \quad (8)$$

We shall always choose the simulator such that $\Delta_1 \gg \|H\|$ in which case $\epsilon \approx \epsilon_1 + \epsilon_2$.

Proof. Suppose H, H_1, H_2 act on Hilbert spaces $\mathcal{H}, \mathcal{H}_1, \mathcal{H}_2$ respectively. Let $N = \dim(\mathcal{H})$ and $N_1 = \dim(\mathcal{H}_1)$. By Lemma 1, the N smallest eigenvalues of H_2 are separated from the rest of the spectrum by a spectral gap at least $\Delta_1 - 2\epsilon_2 > 0$. Thus the low-energy subspace $\mathcal{L}_N(H_2)$ is well defined. Let $\tilde{\mathcal{E}}_2 : \mathcal{H}_1 \rightarrow \mathcal{H}_2$ be an isometry satisfying properties (S1–S3) for a simulator (H_2, \mathcal{E}_2) and a target Hamiltonian H_1 with an error (η_2, ϵ_2) . By definition, $\tilde{\mathcal{E}}_2$ maps \mathcal{H}_1 to the low-energy subspace $\mathcal{L}_{N_1}(H_2)$. First, let us show that $\tilde{\mathcal{E}}_2$ approximately maps $\mathcal{L}_N(H_1)$ to $\mathcal{L}_N(H_2)$. More precisely, we claim that there exists a unitary operator $U : \mathcal{L}_{N_1}(\mathcal{H}_2) \rightarrow \mathcal{L}_{N_1}(\mathcal{H}_2)$ such that

$$\mathcal{L}_N(H_2) = U \tilde{\mathcal{E}}_2 \cdot \mathcal{L}_N(H_1) \quad \text{and} \quad \|U - I\| \leq 2\sqrt{2}\Delta_1^{-1}\epsilon_2. \quad (9)$$

Indeed, let $P_N(H_i)$ be the projector onto the low-energy subspace $\mathcal{L}_N(H_i)$, where $i = 1, 2$. Consider a perturbation $V = \tilde{\mathcal{E}}_2^\dagger H_2 \tilde{\mathcal{E}}_2 - H_1$. Note that $\mathcal{L}_N(H_1 + V) = \tilde{\mathcal{E}}_2^\dagger \cdot \mathcal{L}_N(H_2)$. Applying Lemma 3.1 of Ref. [28] with an unperturbed Hamiltonian H_1 and a perturbation V one gets

$$\|P_N(H_1) - \tilde{\mathcal{E}}_2^\dagger P_N(H_2) \tilde{\mathcal{E}}_2\| \leq \frac{2\|\tilde{\mathcal{E}}_2^\dagger H_2 \tilde{\mathcal{E}}_2 - H_1\|}{\Delta_1} \leq \frac{2\epsilon_2}{\Delta_1}. \quad (10)$$

Taking into account that $\mathcal{L}_N(H_2) \subseteq \mathcal{L}_{N_1}(H_2) = \text{Im}(\tilde{\mathcal{E}}_2)$ one gets

$$\|\tilde{\mathcal{E}}_2 P_N(H_1) \tilde{\mathcal{E}}_2^\dagger - P_N(H_2)\| = \|P_N(H_1) - \tilde{\mathcal{E}}_2^\dagger P_N(H_2) \tilde{\mathcal{E}}_2\|$$

and thus

$$\|\tilde{\mathcal{E}}_2 P_N(H_1) \tilde{\mathcal{E}}_2^\dagger - P_N(H_2)\| \leq \frac{2\epsilon_2}{\Delta_1}. \quad (11)$$

For brevity denote

$$P \equiv \tilde{\mathcal{E}}_2 P_N(H_1) \tilde{\mathcal{E}}_2^\dagger \quad \text{and} \quad Q \equiv P_N(H_2).$$

By Jordan's lemma, there exists an orthonormal basis such that the projectors P and Q are block-diagonal in this basis with all blocks being either 1×1 or 2×2 projectors. Assuming that $2\Delta_1^{-1}\epsilon_2 < 1$ one has $\|P - Q\| < 1$ which implies that all 1×1 blocks of P and Q are the same. Consider some 2×2 block. Without loss of generality, the restrictions of P and Q onto this block have a form

$$P = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \quad \text{and} \quad Q = \begin{bmatrix} c^2 & cs \\ cs & s^2 \end{bmatrix}$$

for some $0 \leq c, s \leq 1$ such that $c^2 + s^2 = 1$. Then $P - Q = s^2 Z - cs X$ and thus $\|P - Q\| = s$. We conclude that $s \leq 2\Delta_1^{-1}\epsilon_2$ for any 2×2 block. Define a unitary

$$U = \begin{bmatrix} c & -s \\ s & c \end{bmatrix} = cI - isY$$

such that $UPU^\dagger = Q$. Note that $\|U - I\| = |c - 1 + is| \leq \sqrt{2}s$. Extending U to the full space $\mathcal{L}_{N_1}(\mathcal{H}_2)$ we obtain $\text{Im}(Q) = U \cdot \text{Im}(P)$ and $\|U - I\| \leq \sqrt{2}s$ which is equivalent to Eq. (9).

Now we are ready to prove that $(H_2, \mathcal{E}_2 \mathcal{E}_1)$ simulates H with a small error. Define an isometry

$$\tilde{\mathcal{E}} = U \tilde{\mathcal{E}}_2 \tilde{\mathcal{E}}_1.$$

Using the first part of Eq. (9) and the fact that $\tilde{\mathcal{E}}_1$ maps \mathcal{H} to the low-energy subspace $\mathcal{L}_N(H_1)$ we conclude that $\tilde{\mathcal{E}}$ maps \mathcal{H} to the low-energy subspace $\mathcal{L}_N(H_2)$. Thus $\tilde{\mathcal{E}}$ obeys property (S1) for the target Hamiltonian H and the simulator $(H_2, \mathcal{E}_2 \mathcal{E}_1)$. Furthermore, the second part of Eq. (9) implies that

$$\eta \equiv \|\tilde{\mathcal{E}} - \mathcal{E}_2 \mathcal{E}_1\| \leq \|U - I\| + \|\tilde{\mathcal{E}}_2 - \mathcal{E}_2\| + \|\tilde{\mathcal{E}}_1 - \mathcal{E}_1\| \leq 2\sqrt{2}\Delta_1^{-1}\epsilon_2 + \eta_2 + \eta_1.$$

Finally, let $H_i^{(N)} = H_i P_N(H_i)$ be the restriction of H_i onto the low-energy subspace $\mathcal{L}_N(H_i)$. Note that $H_1 \tilde{\mathcal{E}}_1 = H_1^{(N)} \tilde{\mathcal{E}}_1$ and $H_2 U \tilde{\mathcal{E}}_2 \tilde{\mathcal{E}}_1 = H_2^{(N)} U \tilde{\mathcal{E}}_2 \tilde{\mathcal{E}}_1$. Thus

$$\|H - \tilde{\mathcal{E}}^\dagger H_2 \tilde{\mathcal{E}}\| \leq \|H - \tilde{\mathcal{E}}_1^\dagger H_1 \tilde{\mathcal{E}}_1\| + \|\tilde{\mathcal{E}}_1^\dagger (H_1^{(N)} - \tilde{\mathcal{E}}_2^\dagger U^\dagger H_2^{(N)} U \tilde{\mathcal{E}}_2) \tilde{\mathcal{E}}_1\|.$$

The first term is upper bounded by ϵ_1 . Thus

$$\|H - \tilde{\mathcal{E}}^\dagger H_2 \tilde{\mathcal{E}}\| \leq \epsilon_1 + \|U \tilde{\mathcal{E}}_2 H_1^{(N)} - H_2^{(N)} U \tilde{\mathcal{E}}_2\|.$$

To bound the second term we write $U = I + M$ and note that

$$\begin{aligned} U \tilde{\mathcal{E}}_2 H_1^{(N)} - H_2^{(N)} U \tilde{\mathcal{E}}_2 &= P_N(H_2)(U \tilde{\mathcal{E}}_2 H_1 - H_2 U \tilde{\mathcal{E}}_2) P_N(H_1) \\ &= P_N(H_2)(\tilde{\mathcal{E}}_2 H_1 - H_2 \tilde{\mathcal{E}}_2) P_N(H_1) + P_N(H_2) M \tilde{\mathcal{E}}_2 H_1^{(N)} \\ &\quad - H_2^{(N)} M \tilde{\mathcal{E}}_2 P_N(H_1). \end{aligned}$$

The norm of the first term is upper bounded by

$$\|\tilde{\mathcal{E}}_2 H_1 - H_2 \tilde{\mathcal{E}}_2\| \leq \|H_1 - \tilde{\mathcal{E}}_2^\dagger H_2 \tilde{\mathcal{E}}_2\| \leq \epsilon_2.$$

Thus

$$\|H - \tilde{\mathcal{E}}^\dagger H_2 \tilde{\mathcal{E}}\| \leq \epsilon_1 + \epsilon_2 + \|U - I\| \cdot \|H_1^{(N)}\| + \|U - I\| \cdot \|H_2^{(N)}\|.$$

Lemma 1 implies that $\|H_2^{(N)}\| \leq \|H_1^{(N)}\| + \epsilon_2$ and $\|H_1^{(N)}\| \leq \|H\| + \epsilon_1$. Combining this and the second part of Eq. (9) one arrives at

$$\|H - \tilde{\mathcal{E}}^\dagger H_2 \tilde{\mathcal{E}}\| \leq \epsilon_1 + \epsilon_2 + O(\Delta_1^{-1} \epsilon_2 \|H\|) + O(\Delta_1^{-1} (\epsilon_2^2 + \epsilon_1 \epsilon_2)).$$

Since we assumed that $\epsilon_1, \epsilon_2 \leq \|H\|$, the last term is at most $O(\Delta_1^{-1} \epsilon_2 \|H\|)$. \square

4. Schrieffer–Wolff Transformation and Perturbative Reductions

Let H be a target Hamiltonian chosen from some particular class of Hamiltonians \mathcal{C} . Suppose our goal is to simulate H with a small error according to Definition 1 using a simulator Hamiltonian H_{sim} which is required to be a member of some smaller class $\mathcal{C}' \subset \mathcal{C}$. Perturbative reductions [2, 22] provide a general method of accomplishing such simulation. Here we describe perturbative reductions based on the Schrieffer–Wolff transformation [26], see for instance [28] and the references therein. Also we provide sufficient conditions under which a k -th order reduction achieves the desired simulation error for $k = 1, 2, 3$, see Lemmas 4–7.

Consider a finite-dimensional Hilbert space \mathcal{H}_{sim} decomposed into a direct sum

$$\mathcal{H}_{\text{sim}} = \mathcal{H}_- \oplus \mathcal{H}_+. \quad (12)$$

Let $N_\pm = \dim(\mathcal{H}_\pm)$ and P_\pm be the projector onto \mathcal{H}_\pm such that $P_- + P_+ = I$. Let O be any linear operator on \mathcal{H}_{sim} . We shall write

$$O_{--} = P_- O P_-, \quad O_{-+} = P_- O P_+, \quad O_{+-} = P_+ O P_-, \quad O_{++} = P_+ O P_+.$$

The operator is said to be block diagonal if $O_{-+} = 0$ and $O_{+-} = 0$. The operator is said to be block off-diagonal if $O_{--} = 0$ and $O_{++} = 0$.

Let H_0 and V be hermitian operators on \mathcal{H}_{sim} such that H_0 is block-diagonal, $(H_0)_{--} = 0$, and such that $(H_0)_{++}$ has all eigenvalues greater or equal to one. Consider a perturbed Hamiltonian

$$H_{\text{sim}} = \Delta H_0 + V, \quad (13)$$

where Δ is a large parameter. We shall always assume that

$$\|V\| < \Delta/2. \quad (14)$$

The Schrieffer–Wolff transformation is a unitary operator on \mathcal{H}_{sim} defined as e^S , where S is an anti-hermitian operator satisfying

$$(e^S H_{\text{sim}} e^{-S})_{-+} = 0, \quad (e^S H_{\text{sim}} e^{-S})_{+-} = 0, \quad S_{--} = 0, \quad S_{++} = 0, \quad \|S\| < \pi/2. \quad (15)$$

In other words, we require that the transformed Hamiltonian $e^S H_{\text{sim}} e^{-S}$ is block diagonal whereas S itself is block off-diagonal. It is known that Eq. (15) has a unique solution S , see Lemma 2.3 and Lemma 3.1 in [28]. In particular, $S = 0$ if $V = 0$. The effective low-energy Hamiltonian H_{eff} is a hermitian operator acting on \mathcal{H}_- defined as

$$H_{\text{eff}} = (e^S H_{\text{sim}} e^{-S})_{--}.$$

Note that $H_{\text{eff}} = 0$ if $V = 0$. Since the operator e^S is unitary and the transformed Hamiltonian $e^S H_{\text{sim}} e^{-S}$ is block-diagonal, each eigenvalue of H_{eff} must be an eigenvalue of H_{sim} . It is known that the i -th smallest eigenvalues of H_{eff} and H_{sim} coincide for all $1 \leq i \leq N_-$, see [28] for details.

Consider now the Taylor series $S = \sum_{j=1}^{\infty} S_j$ and $H_{\text{eff}} = \sum_{j=1}^{\infty} H_{\text{eff},j}$, where S_j and $H_{\text{eff},j}$ are the Taylor coefficients proportional to the j -th power of V . We shall only need the Taylor coefficients

$$H_{\text{eff},1} = V_{--}, \quad (16)$$

$$H_{\text{eff},2} = -\Delta^{-1} V_{-+} H_0^{-1} V_{+-} \quad (17)$$

and

$$H_{\text{eff},3} = \Delta^{-2} V_{-+} H_0^{-1} V_{++} H_0^{-1} V_{+-} - \frac{\Delta^{-2}}{2} (V_{-+} H_0^{-2} V_{+-} V_{--} + \text{h.c.}), \quad (18)$$

see Section 3.2 of [28] for the derivation. Note that the restriction of H_0^{-1} to the subspace \mathcal{H}_+ is well-defined since all eigenvalues of $(H_0)_{++}$ are at least one. It is known that the series for S and H_{eff} converge absolutely for $\|V\| < \Delta/16$ and the j -th Taylor coefficients are bounded as

$$\|S_j\| \leq (b\Delta)^{-j} \|V\|^j \quad \text{and} \quad \|H_{\text{eff},j}\| \leq (c\Delta)^{1-j} \|V\|^j \quad (19)$$

for some constant coefficients $b, c > 0$, see Lemma 3.4 in [28]. Define the k -th order effective Hamiltonian as the truncated series

$$H_{\text{eff}}(k) = \sum_{j=1}^k H_{\text{eff},j}. \quad (20)$$

The above implies that for any $k = O(1)$ and $\|V\| < \Delta \cdot \min\{b, c\}$ one has

$$\|S\| \leq \sum_{j=1}^{\infty} (b\Delta)^{-j} \|V\|^j = O(\Delta^{-1} \|V\|) \quad (21)$$

and

$$\|H_{\text{eff}} - H_{\text{eff}}(k)\| \leq \sum_{j=k+1}^{\infty} (c\Delta)^{1-j} \|V\|^j = O(\Delta^{-k} \|V\|^{k+1}). \quad (22)$$

Suppose now that H_{target} is a fixed target Hamiltonian acting on some Hilbert space $\mathcal{H}_{\text{target}}$ and $\mathcal{E} : \mathcal{H}_{\text{target}} \rightarrow \mathcal{H}_{\text{sim}}$ is some fixed isometry (encoding) such that $\text{Im}(\mathcal{E}) = \mathcal{H}_-$. Define a *logical target Hamiltonian* acting on \mathcal{H}_- as

$$\overline{H}_{\text{target}} = \mathcal{E} H_{\text{target}} \mathcal{E}^\dagger. \quad (23)$$

The goal of perturbative reductions is to approximate $\overline{H}_{\text{target}}$ by the effective low-energy Hamiltonian $H_{\text{eff}}(k)$ emerging from the simulator Hamiltonian H_{sim} defined in Eq. (13), where the parameter Δ controls the approximation error. Below we outline a general strategy for constructing the simulator Hamiltonian proposed by Oliveira and Terhal [2]. The strategy depends on the order k of a reduction.

For first-order reductions one just needs to choose V such that $\overline{H}_{\text{target}} = (V)_{--}$, see Eq. (16). For second-order reductions the perturbation V will be chosen as

$$V = \Delta^{1/2} V_{\text{main}} + V_{\text{extra}}, \quad (24)$$

where $(V_{\text{main}})_{--} = 0$ and V_{extra} is block-diagonal. Both operators V_{main} and V_{extra} are independent of Δ . Substituting V into Eqs. (16, 17) gives

$$H_{\text{eff},1} = (V_{\text{extra}})_{--} \quad \text{and} \quad H_{\text{eff},2} = -(V_{\text{main}})_{-+} H_0^{-1} (V_{\text{main}})_{+-}. \quad (25)$$

We shall choose V_{main} such that $H_{\text{eff},2}$ generates the desired logical target Hamiltonian and, may be, some unwanted terms. The purpose of V_{extra} is to cancel the unwanted terms. In addition, V_{extra} may include all the terms of the target Hamiltonian that are members of the simulator class, such as two-qubit diagonal interactions. Note that the latter belong to all the classes listed in Table 2. Most of the second-order reductions described below will achieve an exact equality $H_{\text{eff},2} = \overline{H}_{\text{target}}$.

For third-order reductions the perturbation V will be chosen as

$$V = \Delta^{2/3} V_{\text{main}} + \Delta^{1/3} \tilde{V}_{\text{extra}} + V_{\text{extra}}, \quad (26)$$

where $(V_{\text{main}})_{--} = 0$, and $V_{\text{extra}}, \tilde{V}_{\text{extra}}$ are block-diagonal. All operators $V_{\text{main}}, V_{\text{extra}}$, and \tilde{V}_{extra} are independent of Δ . Substituting V into Eqs. (16–18) gives

$$H_{\text{eff},1} = \Delta^{1/3} (\tilde{V}_{\text{extra}})_{--} + (V_{\text{extra}})_{--}, \quad H_{\text{eff},2} = -\Delta^{1/3} (V_{\text{main}})_{-+} H_0^{-1} (V_{\text{main}})_{+-}, \quad (27)$$

and

$$H_{\text{eff},3} = (V_{\text{main}})_{-+} H_0^{-1} (V_{\text{main}})_{++} H_0^{-1} (V_{\text{main}})_{+-} + O(\Delta^{-1/3} \|\tilde{V}_{\text{extra}}\| \cdot \|V_{\text{main}}\|^2). \quad (28)$$

We shall choose Δ large enough so that the last term in Eq. (28) can be neglected. We shall choose V_{main} such that $H_{\text{eff},3}$ generates the desired logical target Hamiltonian and, may be, some unwanted terms. The purpose of V_{extra} is to cancel the unwanted terms. In addition, V_{extra} may include all the terms of the target Hamiltonian that are members of the simulator class. Finally, the purpose of \tilde{V}_{extra} is to cancel the second-order term $H_{\text{eff},2}$. Accordingly, we shall always choose \tilde{V}_{extra} such that

$$(\tilde{V}_{\text{extra}})_{--} = (V_{\text{main}})_{-+} H_0^{-1} (V_{\text{main}})_{+-}. \quad (29)$$

Our proof will only use reductions of the order $k = 1, 2, 3$. The following lemmas provide sufficient conditions under which a k -th order reduction achieves a desired simulation error. Recall that our definition of a simulation depends on a particular encoding \mathcal{E} , see Definition 1. The lemmas stated below apply to any fixed encoding \mathcal{E} and the logical target Hamiltonian defined by Eq. (23). In Lemmas 4–6 we assume that H_0 is block-diagonal, $(H_0)_{--} = 0$, and $(H_0)_{++}$ has all eigenvalues greater or equal to 1.

Lemma 4 (First-order reduction). *Suppose one can choose H_0, V such that*

$$\|\bar{H}_{\text{target}} - (V)_{--}\| \leq \epsilon/2. \quad (30)$$

Then $H_{\text{sim}} = \Delta H_0 + V$ simulates H_{target} with an error (η, ϵ) , provided that $\Delta \geq O(\epsilon^{-1}\|V\|^2 + \eta^{-1}\|V\|)$.

Proof. Let $\mathcal{E} : \mathcal{H}_{\text{target}} \rightarrow \mathcal{H}_{\text{sim}}$ be the chosen encoding. Recall that $\text{Im}(\mathcal{E}) = \mathcal{H}_-$. Let us check that $\tilde{\mathcal{E}} = e^{-S}\mathcal{E}$ satisfies conditions (S1–S3) of Definition 1. By definition of the Schrieffer–Wolff transformation, e^{-S} maps \mathcal{H}_- to the low-energy subspace of H_{sim} . Thus $\tilde{\mathcal{E}}$ maps $\mathcal{H}_{\text{target}}$ to the low-energy subspace of H_{sim} which proves (S1). From Eq. (22) one infers that $\|H_{\text{eff}} - H_{\text{eff},1}\| \leq O(\Delta^{-1}\|V\|^2) \leq \epsilon/2$. Combining this and Eq. (30) gives $\|\bar{H}_{\text{target}} - H_{\text{eff}}\| \leq \epsilon$ and thus $\|H_{\text{target}} - \mathcal{E}^\dagger H_{\text{eff}} \mathcal{E}\| \leq \epsilon$. Substituting $H_{\text{eff}} = (e^S H_{\text{sim}} e^{-S})_{--}$ one gets $\|H_{\text{target}} - \tilde{\mathcal{E}}^\dagger H_{\text{sim}} \tilde{\mathcal{E}}\| \leq \epsilon$ which proves condition (S2). Finally, Eq. (21) leads to $\|\mathcal{E} - \tilde{\mathcal{E}}\| = \|I - e^{-S}\| = O(\|S\|) = O(\Delta^{-1}\|V\|) \leq \eta$. This proves condition (S3). \square

Lemma 5 (Second-order reduction). *Suppose one can choose $H_0, V_{\text{main}}, V_{\text{extra}}$ such that V_{extra} is block-diagonal, $(V_{\text{main}})_{--} = 0$, and*

$$\|\bar{H}_{\text{target}} - (V_{\text{extra}})_{--} + (V_{\text{main}})_{-+} H_0^{-1} (V_{\text{main}})_{+-}\| \leq \epsilon/2. \quad (31)$$

Suppose the norm of $V_{\text{main}}, V_{\text{extra}}$ is at most Λ . Then $H_{\text{sim}} = \Delta H_0 + \Delta^{1/2} V_{\text{main}} + V_{\text{extra}}$ simulates H_{target} with an error (η, ϵ) provided that $\Delta \geq O(\epsilon^{-2}\Lambda^6 + \eta^{-2}\Lambda^2)$.

Proof. Let $V = \Delta^{1/2} V_{\text{main}} + V_{\text{extra}}$. By assumption, V has norm $O(\Delta^{1/2}\Lambda)$. Substituting this into Eq. (22) gives $\|H_{\text{eff}} - H_{\text{eff}}(2)\| \leq O(\Delta^{-2}\|V\|^3) = O(\Delta^{-1/2}\Lambda^3) \leq \epsilon/2$. From Eqs. (25, 31) one gets $\|\bar{H}_{\text{target}} - H_{\text{eff}}(2)\| \leq \epsilon/2$ which gives $\|H_{\text{eff}} - \bar{H}_{\text{target}}\| \leq \epsilon$. Finally, Eq. (21) leads to $\|\mathcal{E} - \tilde{\mathcal{E}}\| = \|I - e^{-S}\| = O(\|S\|) = O(\Delta^{-1}\|V\|) = O(\Delta^{-1/2}\Lambda) \leq \eta$. The rest of the proof is identical to the one of Lemma 4. \square

Lemma 6 (Third-order reduction). *Suppose one can choose $H_0, V_{\text{main}}, V_{\text{extra}}, \tilde{V}_{\text{extra}}$ such that $V_{\text{extra}}, \tilde{V}_{\text{extra}}$ are block-diagonal, $(V_{\text{main}})_{--} = 0$,*

$$\|\bar{H}_{\text{target}} - (V_{\text{extra}})_{--} - (V_{\text{main}})_{-+} H_0^{-1} (V_{\text{main}})_{++} H_0^{-1} (V_{\text{main}})_{+-}\| \leq \epsilon/2, \quad (32)$$

and

$$(\tilde{V}_{\text{extra}})_{--} = (V_{\text{main}})_{-+} H_0^{-1} (V_{\text{main}})_{+-}. \quad (33)$$

Suppose the norm of $V_{\text{main}}, V_{\text{extra}}, \tilde{V}_{\text{extra}}$ is at most Λ . Then $H_{\text{sim}} = \Delta H_0 + \Delta^{2/3} V_{\text{main}} + \Delta^{1/3} \tilde{V}_{\text{extra}} + V_{\text{extra}}$ simulates H_{target} with an error (η, ϵ) provided that $\Delta \geq O(\epsilon^{-3}\Lambda^{12} + \eta^{-3}\Lambda^3)$.

Proof. Let $V = \Delta^{2/3} V_{\text{main}} + \Delta^{1/3} \tilde{V}_{\text{extra}} + V_{\text{extra}}$. By assumption, V has norm $O(\Delta^{2/3}\Lambda)$. Substituting this into Eq. (22) gives $\|H_{\text{eff}} - H_{\text{eff}}(3)\| \leq O(\Delta^{-3}\|V\|^4) = O(\Delta^{-1/3}\Lambda^4) \leq \epsilon/4$. Combining Eqs. (27, 28) and Eqs. (32, 33) one gets

$$\|\bar{H}_{\text{target}} - H_{\text{eff}}(3)\| \leq \epsilon/4 + O(\Delta^{-1/3}\|\tilde{V}_{\text{extra}}\| \cdot \|V_{\text{main}}\|^2) = \epsilon/4 + O(\Delta^{-1/3}\Lambda^3) \leq \epsilon/2.$$

This gives $\|H_{\text{eff}} - \bar{H}_{\text{target}}\| \leq \epsilon$. Finally, Eq. (21) leads to $\|\mathcal{E} - \tilde{\mathcal{E}}\| = \|I - e^{-S}\| = O(\|S\|) = O(\Delta^{-1}\|V\|) = O(\Delta^{-1/3}\Lambda) \leq \eta$. The rest of the proof is identical to the one of Lemma 4. \square

The above framework covers all our reductions except for the one described in Sect. 5, namely, the reduction from TIM on degree-3 graphs to TIM on general graphs. The latter is a first-order reduction where the Hamiltonian H_0 is chosen as the one-dimensional TIM. In this case H_0 has only approximately degenerate ground subspace, $(H_0)_{--} \neq 0$, and the rules Eqs. (16–18) for computing the effective Hamiltonian no longer apply. The following is a simple generalization of Lemma 4.

Lemma 7 (Generalized first-order reduction). *Suppose one can choose H_0, V such that H_0 is block-diagonal, $(H_0)_{++}$ has all eigenvalues at least Δ , and $(H_0)_{--}$ has all eigenvalues in the interval $[-\Delta/2, \Delta/2]$. Suppose also that*

$$\|\overline{H}_{\text{target}} - (H_0)_{--} - (V)_{--}\| \leq \epsilon/2. \quad (34)$$

Then $H_{\text{sim}} = H_0 + V$ simulates H_{target} with an error (η, ϵ) provided that $\Delta \geq O(\epsilon^{-1} \|V\|^2 + \eta^{-1} \|V\|)$.

Proof. We can use the same arguments as in the proof of Lemma 4 except that now H_{eff} has a 0-th order term $H_{\text{eff},0} = (H_0)_{--}$. By assumption, the unperturbed Hamiltonian H_0 has an energy gap at least $\Delta/2$ separating \mathcal{H}_- and \mathcal{H}_+ . Lemma 3.4 of Ref. [28] implies that the series for S and H_{eff} converges absolutely for $\|V\| < \Delta/32$ and the Taylor coefficients S_j and $H_{\text{eff},j}$ are bounded as in Eqs. (21, 22). Therefore $\|H_{\text{eff}} - H_{\text{eff},0} - H_{\text{eff},1}\| \leq O(\Delta^{-1} \|V\|^2)$ and $\|S\| \leq O(\Delta^{-1} \|V\|)$. The rest of the proof is the same as in Lemma 4. \square

5. Reduction from Degree-3 Graphs to General Graphs

Consider a target Hamiltonian H_{target} describing the TIM on n qubits. We assume that each qubit can be coupled to any other qubit with ZZ interactions. Below we show how to simulate H_{target} using TIM with interactions of degree 3. Let us first informally sketch the main idea. We shall encode each qubit u of the target model into the ground subspace of a TIM Hamiltonian on a one-dimensional chain L_u of some length m . The chain will be in the ferromagnetic phase such that the ground states ψ_0 and ψ_1 originating from the two different \mathbb{Z}_2 -symmetry sectors are approximately degenerate forming one logical qubit. The basis states of the logical qubit will be defined as $|\overline{0}\rangle \sim |\psi_0\rangle + |\psi_1\rangle$ and $|\overline{1}\rangle \sim |\psi_0\rangle - |\psi_1\rangle$. Important parameters of the logical qubit are the energy splitting δ between ψ_0 and ψ_1 and the energy gap Δ separating ψ_0, ψ_1 from excited states. We shall work in the regime $\delta \geq \text{poly}(1/m)$ and $\Delta/\delta \geq \text{poly}(m)$ which can be achieved if the chain is sufficiently close to the quantum phase transition point. The logical Pauli operator \overline{X}_u will be simulated by the energy splitting between ψ_0 and ψ_1 . The logical Pauli operator \overline{Z}_u will be simulated by applying a magnetic field hZ_i to an arbitrarily chosen qubit $i \in L_u$. The strength of the field h will be much smaller than the gap Δ to enable a perturbative analysis. We shall only need the first-order perturbation theory. Since the one-dimensional TIM is exactly solvable, all parameters of the logical qubit will be efficiently computable. Assuming that the target model has n qubits, the simulator model will be composed of n chains L_1, \dots, L_n of length m each. We can simulate a logical interaction $\overline{Z}_u \overline{Z}_v$ by choosing an arbitrary pair of qubits $i \in L_u, j \in L_v$ and applying the Ising interaction $Z_i Z_j$. Since each logical qubit L_u is coupled to at most $n-1$ other logical qubits, choosing $m \geq n-1$ guarantees that each qubit of L_u is coupled to at most one qubit from a different chain. In addition, each qubit of L_u must be coupled to its left and right neighbors in L_u . Thus the simulator model has interactions of degree

3. A logical transverse field \overline{X}_u is automatically simulated due to the ground state energy splitting of L_u . Thereby, we shall be able to simulate any logical TIM Hamiltonian.

Let us now describe the reduction formally. For the sake of clarity, we begin by constructing a single logical qubit. Consider a chain of m qubits with periodic boundary conditions. Qubits will be labeled by elements of the cyclic group $j \in \mathbb{Z}_m$. Consider a TIM Hamiltonian

$$H_{\text{chain}} = -g \sum_{j \in \mathbb{Z}_m} Z_j Z_{j+1} - \sum_{j \in \mathbb{Z}_m} X_j, \quad (35)$$

where

$$g = 1 + \frac{c \log(m)}{m} \quad (36)$$

for some parameter $c \gg 1$ to be chosen later. The Hamiltonian H_{chain} can be diagonalized via the Jordan–Wigner transformation and all its eigenvalues have been explicitly computed [14]. Let the three smallest eigenvalues of H_{chain} be $E_0 \leq E_1 \leq E_2$. We shall use the following well-known fact [29, 34].

Fact 1. Let $\omega_m = e^{2\pi i/m}$ be the m -th root of unity. For any $g > 1$ one has

$$E_0 = - \sum_{j \in \mathbb{Z}_m} |g - \omega_m^{j+1/2}|, \quad E_1 = - \sum_{j \in \mathbb{Z}_m} |g - \omega_m^j|, \quad E_2 = E_0 + 4|g - \omega_m^{1/2}|. \quad (37)$$

Furthermore, the eigenvalues E_0, E_1 have multiplicity one and the corresponding eigenvectors ψ_0, ψ_1 satisfy $X^{\otimes m} \psi_0 = \psi_0$ and $X^{\otimes m} \psi_1 = -\psi_1$.

Let $\mathcal{H} = (\mathbb{C}^2)^{\otimes m}$ be the full Hilbert space of n qubits. Define an encoding $\mathcal{E} : \mathbb{C}^2 \rightarrow \mathcal{H}$ as

$$\mathcal{E}|0\rangle \equiv |\overline{0}\rangle = (|\psi_0\rangle + |\psi_1\rangle)/\sqrt{2} \quad \text{and} \quad \mathcal{E}|1\rangle \equiv |\overline{1}\rangle = (|\psi_0\rangle - |\psi_1\rangle)/\sqrt{2}. \quad (38)$$

Thus we identify the states ψ_0 and ψ_1 with the states $|+\rangle$ and $|-\rangle$ of the logical qubit. Decompose $\mathcal{H} = \mathcal{H}_- \oplus \mathcal{H}_+$, where \mathcal{H}_- is the logical subspace spanned by ψ_0, ψ_1 and \mathcal{H}_+ is the orthogonal complement of \mathcal{H}_- . Then H_{chain} is block-diagonal. Performing the overall energy shift by $(E_0 + E_1)/2$ we arrive at

$$(H_{\text{chain}})_{--} = -\delta \overline{X} \quad \text{and} \quad (H_{\text{chain}})_{++} \geq \Delta I, \quad (39)$$

where $\overline{X} = \mathcal{E} X \mathcal{E}^\dagger = |\psi_0\rangle\langle\psi_0| - |\psi_1\rangle\langle\psi_1|$ is the logical Pauli X operator,

$$\delta = (E_1 - E_0)/2 \quad \text{and} \quad \Delta = 4|g - \omega_m^{1/2}| - \delta.$$

Note that δ and Δ can be computed in time $\text{poly}(m)$ using Eq. (37). In Appendix A we prove that

$$\Omega(m^{-c-3/2}) \leq \delta \leq O(m^{-c-1/2}) \quad (40)$$

in the limit $m \rightarrow \infty$. Therefore

$$\Delta \geq \frac{4c \log(m)}{m} - O(m^{-1}) - O(m^{-c-1/2}) \geq \Omega(m^{-1}). \quad (41)$$

By choosing the constant c sufficiently large we can make the ratio Δ/δ bigger than any fixed polynomial of m and, at the same time, keep δ at least polynomial in $1/m$.

Consider now a perturbation $V = hZ_j$, where $|h| \ll \Delta$ and $j \in \mathbb{Z}_m$ is an arbitrarily chosen qubit. The first-order effective Hamiltonian acting on \mathcal{H}_- is $h(Z_j)_{--}$. To compute $(Z_j)_{--}$ we need to know matrix elements $\langle \psi_\alpha | Z_j | \psi_\beta \rangle$ for $\alpha, \beta = 0, 1$. Note that Z_j anti-commutes with $X^{\otimes m}$. Using Fact 1 we infer that $\langle \psi_0 | Z_j | \psi_0 \rangle = 0$ and $\langle \psi_1 | Z_j | \psi_1 \rangle = 0$. Therefore $(Z_j)_{--}$ must be a linear combination of the logical Pauli operators \bar{Z} and \bar{Y} . Since H_{chain} has real matrix elements in the standard basis, the same is true for the restrictions of H_{chain} onto the sectors $X^{\otimes m} = \pm 1$. Therefore ψ_0 and ψ_1 must have real amplitudes in the standard basis. This shows that $\langle \psi_0 | Z_j | \psi_1 \rangle$ must be real and thus

$$(Z_j)_{--} = \xi \bar{Z}, \quad \text{where } \xi \equiv \langle \psi_1 | Z_j | \psi_0 \rangle \quad (42)$$

and $\bar{Z} = \mathcal{E}Z\mathcal{E}^\dagger = |\psi_0\rangle\langle\psi_1| + |\psi_1\rangle\langle\psi_0|$ is the logical Pauli Z operator. It can be easily shown that ξ does not depend on the choice of j . We shall need the following expression for ξ computed in Ref. [29], see Eq. (77) therein.

Fact 2. *Suppose $g > 1$. Let $\epsilon_p \equiv |g - \omega_m^p|$, where p is either integer or half-integer. Then*

$$|\xi| = \frac{(1 - g^{-2})^{1/8} \prod_{p \in \mathbb{Z}_m} \prod_{q \in \mathbb{Z}_m + 1/2} (\epsilon_p + \epsilon_q)^{1/4}}{\prod_{p, p' \in \mathbb{Z}_m} (\epsilon_p + \epsilon_{p'})^{1/8} \prod_{q, q' \in \mathbb{Z}_m + 1/2} (\epsilon_q + \epsilon_{q'})^{1/8}} \quad (43)$$

Furthermore, in Appendix A we prove that ξ is positive and

$$\xi \geq (1 - g^{-2})^{1/8} \geq \Omega(m^{-1/8}) \quad (44)$$

for all $m \geq 2$ and for all $g > 1$. Note that ξ can be computed in time $\text{poly}(m)$ using Eq. (43). We can now simulate any target Hamiltonian on a single qubit which has a form

$$H_{\text{target}} = -h^x X + h^z Z, \quad h^x \geq 0. \quad (45)$$

Let $J = \max(|h^z|, h^x)$ be the interaction strength of H_{target} . Choose the simulator Hamiltonian as

$$H_{\text{sim}} = H_0 + V, \quad H_0 = h^x \delta^{-1} H_{\text{chain}}, \quad V = h^z \xi^{-1} Z_j. \quad (46)$$

Here $j \in \mathbb{Z}_m$ is an arbitrary qubit. From Eqs. (39, 42) we infer that the first-order effective Hamiltonian acting on \mathcal{H}_- is

$$H_{\text{eff}}(1) = (H_{\text{sim}})_{--} = h^x \delta^{-1} (H_{\text{chain}})_{--} + h^z \xi^{-1} (Z_j)_{--} = -h^x \bar{X} + h^z \bar{Z} = \bar{H}_{\text{target}}.$$

Note that H_0 has an energy gap $\Delta' = h^x \Delta \delta^{-1}$ separating \mathcal{H}_- and \mathcal{H}_+ . By Lemma 7, the Hamiltonian H_{sim} and the encoding \mathcal{E} simulate H_{target} with an error (η, ϵ) provided that $\Delta' \geq \text{poly}(h^z \xi^{-1}, \epsilon^{-1}, \eta^{-1})$ for some constant degree polynomial. We can assume without loss of generality that $h^x \geq \epsilon/2$ since we only need to approximate the target Hamiltonian with an error $\epsilon/2$, see Lemma 7. Then $\Delta' \geq \Omega(\epsilon m^{-1} \delta^{-1})$. Here we used the bound $\Delta = \Omega(m^{-1})$, see Eq. (41). Since $|h^z| \leq J$, we have to satisfy $\delta^{-1} \geq \text{poly}(m, J, \xi^{-1}, \epsilon^{-1}, \eta^{-1})$. Since $\xi^{-1} = O(m^{1/8})$, see Eq. (44), this is equivalent to $\delta^{-1} \geq \text{poly}(m, J, \epsilon^{-1}, \eta^{-1})$. This can always be achieved by choosing a large enough

constant c in Eq. (36) since $\delta^{-1} = \Omega(m^{c+3/2})$, see Eq. (40). Finally, we express δ^{-1} in terms of the interaction strength J' of the simulator Hamiltonian. From Eq. (46) one gets $J' = O(h^x \delta^{-1})$ and thus we can achieve a simulation error (η, ϵ) by choosing $J' = \text{poly}(m, J, \epsilon^{-1}, \eta^{-1})$.

Consider now a target Hamiltonian on n qubits which has a form

$$H_{\text{target}} = \sum_{0 \leq u < v \leq n-1} \omega_{u,v} Z_u Z_v + \sum_{u=0}^{n-1} h_u^z Z_u - h_u^x X_u. \quad (47)$$

Without loss of generality $h_u^x \geq 0$ (otherwise, conjugate the Hamiltonian by Z_u). We shall encode each qubit u into a chain L_u of length $m = n$ as defined above. Let $H_{\text{chain}}^{(u)}$ be the Hamiltonian Eq. (35) describing the chain L_u . We shall arrange the chains into a square grid of size $n \times n$ such that a cell (u, i) of the grid represents the i -th qubit of the chain L_u . Here $0 \leq u, i \leq n-1$. All chains use the same parameter g . Choose the simulator Hamiltonian as

$$H_{\text{sim}} = H_0 + V, \quad H_0 = \delta^{-1} \sum_{u=0}^{n-1} h_u^x H_{\text{chain}}^{(u)}, \quad (48)$$

$$V = \xi^{-2} \sum_{0 \leq u < v \leq n-1} \omega_{u,v} Z_{(u,v)} Z_{(v,u)} + \xi^{-1} \sum_{u=0}^{n-1} h_u^z Z_{(u,0)}. \quad (49)$$

Note that H_{sim} is a TIM Hamiltonian acting on n^2 qubits and such that each qubit is coupled to at most three other qubits with ZZ interactions. Namely, a qubit (u, v) is coupled only to the qubits $(u, v \pm 1)$ and (v, u) . Let \mathcal{H}_- be the n -fold tensor product of the two-dimensional logical subspaces describing each chain L_u . The above analysis for a single logical qubit shows that $(H_{\text{chain}}^{(u)})_{--} = -\delta \bar{X}_u$ and $(Z_{(u,v)})_{--} = \xi \bar{Z}_u$ for any qubit v in the chain L_u . Therefore the first-order effective Hamiltonian acting on \mathcal{H}_- is

$$H_{\text{eff}}(1) = (H_{\text{sim}})_{--} = \sum_{0 \leq u < v \leq n-1} \omega_{u,v} \bar{Z}_u \bar{Z}_v + \sum_{u=0}^{n-1} h_u^z \bar{Z}_u - h_u^x \bar{X}_u = \bar{H}_{\text{target}}, \quad (50)$$

where the encoding \mathcal{E} is the n -fold tensor product of single qubit encodings defined in Eq. (38).

Let (η, ϵ) be the desired simulation error and J be the maximum magnitude of the coefficients in H_{target} . We can assume without loss of generality that $h_u^x \geq \epsilon/2n$ for all u . Then the energy gap of H_0 separating \mathcal{H}_- from excited states is $\Delta' \geq \epsilon \delta^{-1} \Delta/2n$, where Δ is the energy gap of a single chain, see Eq. (39). By Lemma 7, the Hamiltonian H_{sim} and the encoding \mathcal{E} simulate H_{target} with an error (η, ϵ) provided that $\Delta' \geq \text{poly}(n, J, \epsilon^{-1}, \eta^{-1})$. This is equivalent to $\delta^{-1} \geq \text{poly}(n, J, \epsilon^{-1}, \eta^{-1})$ (use the same bounds as above), which can always be satisfied by choosing a large enough constant c in Eq. (36). Then the simulator Hamiltonian has interaction strength $J' = O(\delta^{-1} J) = \text{poly}(n, J, \epsilon^{-1}, \eta^{-1})$.

To conclude, we have shown that any Hamiltonian $H_{\text{target}} \in \text{TIM}(n, J)$ can be simulated with an error (η, ϵ) by a Hamiltonian $H_{\text{sim}} \in \text{TIM}(n^2, J')$ such that $J' = \text{poly}(n, J, \epsilon^{-1}, \eta^{-1})$ and H_{sim} has interaction degree 3. The simulation uses the encoding \mathcal{E} defined in Eq. (38). Furthermore, the coefficients of H_{sim} can be computed in time $\text{poly}(n)$.

6. Reduction from TIM to Dimers

In this section we construct a TIM simulator for the hard-core dimer model. It involves a composition of a first-order and a second-order reduction. First let us construct a classical Ising Hamiltonian H_0 composed of terms proportional to n_u and $n_u n_v$ such that ground states of H_0 are m -dimers. Consider a graph $G = (U, E)$ with n nodes. Define operators

$$N_U = \sum_{u \in U} n_u \quad \text{and} \quad N_E = \sum_{(u,v) \in E} n_u n_v. \quad (51)$$

These operators act on the full Hilbert space $\mathcal{B} \cong (\mathbb{C}^2)^{\otimes n}$. Define

$$H_0 = N_U - 2N_E + \Gamma \sum_{D(u,v)=2} n_u n_v, \quad \Gamma > 2|E|. \quad (52)$$

Here $D(u, v)$ denotes the graph distance between nodes u, v . Note that H_0 is a TIM Hamiltonian (with a zero transverse field).

Lemma 8. *The Hamiltonian H_0 has zero ground state energy and its ground subspace is spanned by m -dimers with $0 \leq m \leq n/2$. Furthermore, if S is an m -dimer and $T = S \setminus u$ for some $u \in S$ then $\langle T | H_0 | T \rangle = 1$.*

Proof. Suppose $S \subseteq U$ is an m -dimer. By definition, any pair of dimers in S is separated by distance at least three. Thus $\langle S | n_u n_v | S \rangle = 0$ whenever $D(u, v) = 2$. Therefore

$$\langle S | H_0 | S \rangle = \langle S | N_U | S \rangle - 2 \langle S | N_E | S \rangle = 2m - 2m = 0.$$

Next consider any subset of nodes S such that $\langle S | H_0 | S \rangle \leq 0$. It suffices to show that S is an m -dimer for some integer m . Indeed, the negative term in H_0 cannot be smaller than $-2|E|$. Since $\Gamma > 2|E|$, the energy of S can be non-positive only if

$$\langle S | n_u n_v | S \rangle = 0 \quad \text{whenever} \quad D(u, v) = 2. \quad (53)$$

Let $S = C_1 \cup \dots \cup C_m$ be the decomposition of S into connected components. Since the graph has no triangles, Eq. (53) implies that each connected component of S is either a single node or a dimer. Therefore

$$0 \geq \langle S | H_0 | S \rangle = \sum_{\alpha=1}^m \langle C_\alpha | N_U - 2N_E | C_\alpha \rangle. \quad (54)$$

Clearly, $\langle C_\alpha | N_U - 2N_E | C_\alpha \rangle = 1$ if C_α is a single node and $\langle C_\alpha | N_U - 2N_E | C_\alpha \rangle = 0$ if C_α is a dimer. Thus Eq. (54) is possible only if all C_α are dimers. From Eq. (53) one infers that the distance between different dimers C_α is at least three. This shows that S is an m -dimer for some m .

Finally, removing any single node u from an m -dimer S transforms one of the connected components C_α into a single node. The above shows that $T = S \setminus u$ has energy $\langle T | H_0 | T \rangle = 1$. \square

Fix any integer $1 \leq m \leq n/2$. Consider a target Hamiltonian $H_{\text{target}} \in \text{HCD}(n, m, J)$ describing the m -dimer sector of the hard-core dimers model on some triangle-free graph $G = (U, E)$ with n nodes, see Eq. (5).

Our first reduction has a simulator Hamiltonian

$$\tilde{H}_{\text{sim}} = \tilde{\Delta} \tilde{H}_0 + \tilde{V}, \quad \tilde{H}_0 = (N_U - 2m)(N_U - 2m + 1), \quad \tilde{V} \in \text{TIM}(n, \tilde{J}). \quad (55)$$

All above operators act on the full Hilbert space \mathcal{B} . The perturbation \tilde{V} will be chosen at the next reduction. Note that \tilde{H}_{sim} is a TIM Hamiltonian. Since eigenvalues of N_U are integers, the ground subspace of \tilde{H}_0 is spanned by subsets of nodes of cardinality $2m$ or $2m - 1$. By Lemma 4, the Hamiltonian \tilde{H}_{sim} can simulate the restriction of any TIM Hamiltonian \tilde{V} onto the subspace $\mathcal{H} \equiv \mathcal{B}_{2m} \oplus \mathcal{B}_{2m-1}$. In the rest of this section we assume that our full Hilbert space is \mathcal{H} .

Our second reduction has a simulator Hamiltonian

$$H_{\text{sim}} = \Delta H_0 + V, \quad V = \Delta^{1/2} V_{\text{main}} + V_{\text{extra}}, \quad (56)$$

where H_0 is the Hamiltonian constructed in Lemma 8,

$$V_{\text{main}} = t^{1/2} \sum_{u \in U} X_u \quad \text{and} \quad V_{\text{extra}} = H_{\text{diag}} + t N_U. \quad (57)$$

Here t and H_{diag} are defined by the target HCD Hamiltonian Eq. (5) and all operators are restricted to the subspace \mathcal{H} with $2m$ or $2m - 1$ particles. Note that H_{sim} is a TIM Hamiltonian. Lemma 8 implies that the ground subspace of H_0 is spanned by m -dimers, that is, $\mathcal{H}_- = \mathcal{D}_m$.

Let us check that the perturbation has all the properties stated in Lemma 5. First, we note that $(V_{\text{main}})_{--} = 0$ since any pair of m -dimers either coincide or differ on at least two nodes. Obviously, V_{extra} is block-diagonal. It remains to check Eq. (31). Let S and S' be arbitrary m -dimers. Then

$$\langle S' | (V_{\text{main}})_{-+} H_0^{-1} (V_{\text{main}})_{+-} | S \rangle = t \sum_{u, v \in U} \langle S' | X_v P_+ H_0^{-1} P_+ X_u | S \rangle. \quad (58)$$

Recall that all operators in Eq. (56) are restricted to the subspace with $2m$ or $2m - 1$ particles. Thus $X_u | S \rangle = 0$ whenever $u \notin S$ since in this case $X_u | S \rangle$ contains $2m + 1$ particles. In the remaining case, $u \in S$, Lemma 8 implies that $X_u | S \rangle$ is an eigenvector of H_0 with the eigenvalue 1, so that $H_0^{-1} X_u | S \rangle = X_u | S \rangle$. Thus

$$\langle S' | (V_{\text{main}})_{-+} H_0^{-1} (V_{\text{main}})_{+-} | S \rangle = t \sum_{u \in S, v \in S'} \langle S' | X_v X_u | S \rangle. \quad (59)$$

The sum over $u = v$ gives a contribution $t |S| \delta_{S, S'} = \langle S | t N_U | S' \rangle$. The sum over $u \neq v$ is non-zero only if S and S' can be obtained from each other by moving one particle from some node u to another node v , in which case $\langle S' | X_v X_u | S \rangle = \langle S' | W_{u, v} | S \rangle$. Thus

$$(V_{\text{main}})_{-+} H_0^{-1} (V_{\text{main}})_{+-} = t N_U + t \sum_{\{u, v\} \in U} W_{u, v} \quad (60)$$

and

$$(V_{\text{extra}})_{--} - (V_{\text{main}})_{-+} H_0^{-1} (V_{\text{main}})_{+-} = -t \sum_{\{u, v\} \in U} W_{u, v} + H_{\text{diag}} = H_{\text{target}}. \quad (61)$$

Thus all conditions of Lemma 5 are satisfied.

To compose the two reductions we extend H_{sim} defined in Eq. (56) to the full Hilbert space \mathcal{B} and substitute $\tilde{V} = H_{\text{sim}}$ into Eq. (55). Combining Lemmas 3, 4, 5 we conclude that any Hamiltonian $H_{\text{target}} \in \text{HCD}(n, m, J)$ can be simulated with an error (ϵ, η) by a Hamiltonian $\tilde{H}_{\text{sim}} \in \text{TIM}(n, J')$ where $J' = \text{poly}(n, J, \epsilon^{-1}, \eta^{-1})$. The simulation uses the trivial encoding $\mathcal{E} : \mathcal{D}_m \rightarrow \mathcal{B}$, that is, $\mathcal{E}|S\rangle = |S\rangle$ for any m -dimer S .

7. Reduction from Dimers to Range-2 Bosons

In this section we construct an HCD simulator for range-2 hard-core bosons. It involves a third-order reduction. Consider a target Hamiltonian $H_{\text{target}} \in \text{HCB}_2(n, m, J)$ describing the m -particle sector of range-2 hard-core bosons on some graph $G = (U, E)$ with n nodes. For the sake of clarity, let us first consider a special case of homogeneous hopping amplitudes, that is,

$$H_{\text{target}} = -t \sum_{(u,v) \in E} W_{u,v} + H_{\text{diag}}, \quad t \geq 0. \quad (62)$$

Recall that H_{target} acts on the Hilbert space $\mathcal{B}_{m,2}(G)$ spanned by 2-sparse subsets of m nodes.

The HCD simulator will be defined on an extended graph $G' = (U', E')$ obtained from G by placing an extra node at the center of every edge of G and attaching an extra hanging edge to every node of G , see Fig. 3 for an example. The extra node located at the center of an edge $(u, v) \in E$ will be denoted³ $u + v$. The extra node attached to a node $u \in U$ by a hanging edge will be denoted u^* . Thus the extended graph G' has a set of nodes

$$U' = U \cup U^* \cup U^+, \quad U^* = \{u^* : u \in U\}, \quad U^+ = \{u + v : u, v \in U \text{ and } (u, v) \in E\}. \quad (63)$$

We shall represent a boson located at a node $u \in U$ by a dimer occupying the subset $\{u, u^*\} \subseteq U'$.

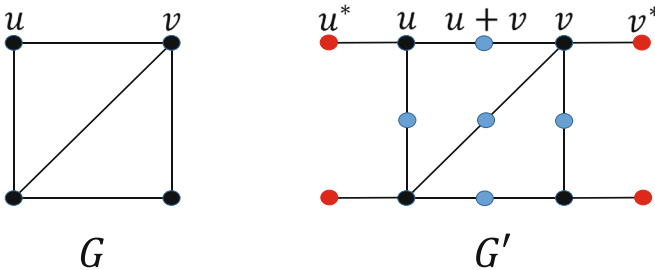


Fig. 3. Construction of the extended graph $G' = (U', E')$ for hard-core dimers starting from the graph $G = (U, E)$ of the hard-core bosons model. The subsets of nodes U^* and U^+ are highlighted in red and blue respectively. A boson located at a node $u \in U$ is represented by a dimer occupying the subset $\{u, u^*\} \subseteq U'$

³ Here the addition is merely a symbol; it has no algebraic meaning.

A simulator HCD Hamiltonian acting on the Hilbert space of m -dimers $\mathcal{D}_m(G')$ is defined as $H_{\text{sim}} = \Delta H_0 + V$, where

$$H_0 = \sum_{w \in U^+} \Delta_w n_w \quad (64)$$

penalizes m -dimers occupying the extra nodes located at the centers of edges of G . For now we set $\Delta_w = 1$ for all $w \in U^+$. We shall need a more general expression for Δ_w in the case of non-homogeneous hopping amplitudes. Clearly, H_0 has zero ground state energy and its ground subspace is spanned by m -dimers $S \subseteq U'$ such that $S \cap U^+ = \emptyset$. The perturbation is defined as $V = \Delta^{2/3} V_{\text{main}} + \Delta^{1/3} \tilde{V}_{\text{extra}} + V_{\text{extra}}$, where

$$V_{\text{main}} = -t^{1/3} \sum_{\{u,v\} \in U'} W_{u,v}, \quad (65)$$

$$\tilde{V}_{\text{extra}} = t^{2/3} \sum_{u \in U} d(u) n_u. \quad (66)$$

$$V_{\text{extra}} = H_{\text{diag}} + t \sum_{u \in U} d_2(u) n_u, \quad (67)$$

For now we define $d(u)$ as the degree of a node u in the original graph G and $d_2(u) \equiv d(u)(d(u) - 1)$. We shall need a more general expression for $d(u)$ and $d_2(u)$ in the case of non-homogeneous hopping amplitudes.

Let us check that the perturbation has all the properties stated in Lemma 6. First, we claim that $(V_{\text{main}})_{--} = 0$. Indeed, suppose $|S\rangle$ is a ground state of H_0 . Then S must be a union of dimers $\{u, u^*\}$ with $u \in U$. Since (u, u^*) is the only edge of G' attached to u^* , the only hopping terms that can map S to some m -dimer S' are those that replace some dimer $\{u, u^*\} \subseteq S$ with a dimer $\{u, u+v\}$ for some $(u, v) \in E$, see Fig. 4. This requires a single hopping from u^* to $u+v$. Then S' has a particle at some node $u+v$ and thus $|S'\rangle$ is an excited state of H_0 . Thus $(V_{\text{main}})_{--} = 0$. The operators V_{extra} and \tilde{V}_{extra} are block-diagonal simply because they are diagonal.

Let us now describe the encoding $\mathcal{E} : \mathcal{B}_{m,2}(G) \rightarrow \mathcal{D}_m(G')$. Recall that $\mathcal{B}_{m,2}(G)$ and $\mathcal{D}_m(G')$ are the Hilbert spaces of the target and the simulator models. Given a 2-sparse subset of nodes $S \subseteq U$ in the graph G let $\mathcal{E}(S) \subseteq U \cup U^*$ be the subset of nodes in the graph G' that includes all nodes $u \in S$ and all nodes u^* such that $u \in S$. Define $\mathcal{E}|S\rangle = |\mathcal{E}(S)\rangle$. Obviously, \mathcal{E} is an isometry. Let us check that $\text{Im}(\mathcal{E})$ coincides with the ground subspace of H_0 . Indeed, suppose $S \subseteq U'$ is a ground state of H_0 , that is, S is an m -dimer in G' such that $S \subseteq U \cup U^*$. Then all dimers in S must have a form $\{u, u^*\}$ for some $u \in U$. Consider any distinct nodes $u, v \in S \cap U$. By definition of an m -dimer, any dimers in S are separated by at least three edges in the graph G' . Then the nodes u and v are separated by at least two edges in the graph G , that is, $S \cap U$ is a 2-sparse subset of m nodes in the graph G . Since $S = \mathcal{E}(S \cap U)$, this shows that S belongs to the image of \mathcal{E} . Conversely, if $S \subseteq U$ is any 2-sparse subset of m nodes in G then $\mathcal{E}(S)$ is an m -dimer in G such that $\mathcal{E}(S) \subseteq U \cup U^*$. This proves that $\text{Im}(\mathcal{E})$ coincides with the ground subspace of H_0 .

Let us now check condition Eq. (32) of Lemma 6. Consider any m -dimer $S \subseteq U'$ such that $S \cap U^+ = \emptyset$. We have already shown that $V_{\text{main}}|S\rangle$ is a superposition of states $|S'\rangle$, where S' is obtained from S by replacing a dimer $\{u, u^*\}$ with a dimer $\{u, u+v\}$ for some $u \in S \cap U$ and $v \in U$ such that $(u, v) \in E$, see Fig. 4. By definition of an m -dimer, $\{u, u^*\}$ is separated from all other dimers of S by at least three edges of the graph G' .

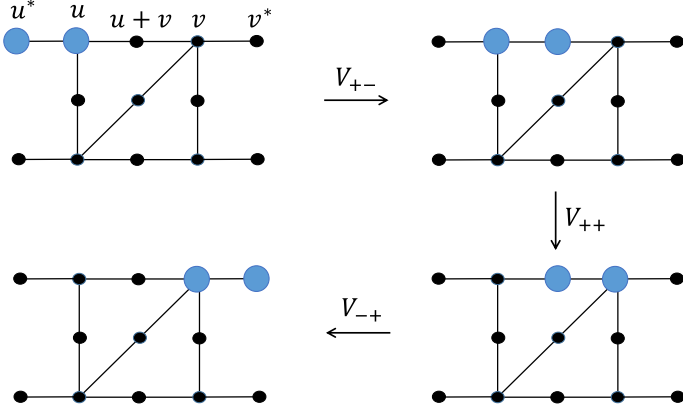


Fig. 4. A third-order process transfers a dimer from $\{u, u^*\}$ to $\{v, v^*\}$. Here $V \equiv V_{\text{main}}$. Since each dimer in G' encodes one particle in G , this process simulates the logical hopping operator $\overline{W}_{u,v}$

However, since $S \cap U^+ = \emptyset$, this is possible only if $\{u, u^*\}$ is separated from all other dimers of S by at least four edges of G' . Then the dimer $\{u, u+v\}$ is separated from all other dimers of S' by at least three edges of G' , that is, S' is an m -dimer. Note also that S' occupies exactly one node of U^+ , that is, $H_0|S'\rangle = |S'\rangle$ and thus $H_0^{-1}|S'\rangle = |S'\rangle$ (recall that we set $\Delta_w = 1$ in the case of homogeneous hopping amplitudes). The above arguments show that

$$(V_{\text{main}})_{+-}|S\rangle = -t^{1/3} \sum_{u \in S \cap U} \sum_{v: (u,v) \in E} W_{u^*, u+v} |S\rangle. \quad (68)$$

Using the above equation one can easily get

$$\begin{aligned} & \langle S' | (V_{\text{main}})_{-+} H_0^{-1} (V_{\text{main}})_{++} H_0^{-1} (V_{\text{main}})_{+-} |S\rangle \\ &= -t \sum_{(u,v) \in E} \langle S' | W_{u+v, v^*} W_{u,v} W_{u^*, u+v} |S\rangle \\ & \quad -t \sum_{(u,v) \neq (u,w) \in E} \langle S' | W_{u+w, u^*} W_{u+v, u+w} W_{u^*, u+v} |S\rangle \end{aligned} \quad (69)$$

Here S' is some m -dimer $S' \subseteq U'$ such that $S' \cap U^+ = \emptyset$. The terms in the first and the second line in the righthand side of Eq. (69) describe triple-hopping processes shown on Figs. 4 and 5 respectively. The former implements a logical hopping operator $\overline{W}_{u,v} = \mathcal{E} W_{u,v} \mathcal{E}^\dagger$, while the latter generates unwanted terms proportional to $\overline{n}_u d(u)(d(u) - 1)$, where $d(u)$ is the degree of u in the graph G . Thus

$$(V_{\text{main}})_{-+} H_0^{-1} (V_{\text{main}})_{++} H_0^{-1} (V_{\text{main}})_{+-} = -t \sum_{(u,v) \in E} \overline{W}_{u,v} - t \sum_{u \in U} d_2(u) \overline{n}_u. \quad (70)$$

Note that the last term is canceled by $(V_{\text{extra}})_{--}$, so that

$$(V_{\text{extra}})_{--} + (V_{\text{main}})_{-+} H_0^{-1} (V_{\text{main}})_{++} H_0^{-1} (V_{\text{main}})_{+-} = \overline{H}_{\text{diag}} - t \sum_{(u,v) \in E} \overline{W}_{u,v} = \overline{H}_{\text{target}}$$

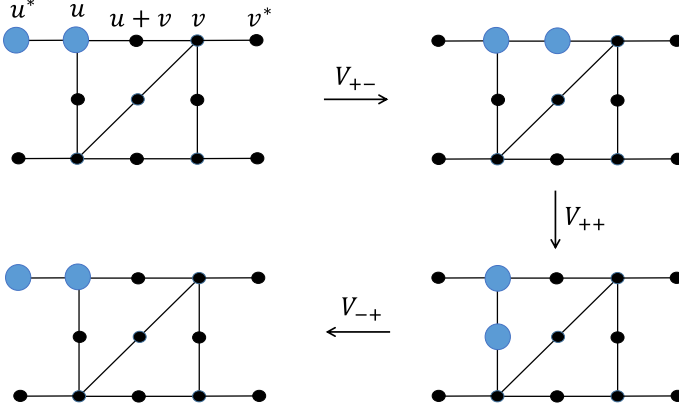


Fig. 5. An unwanted third-order process transfers a dimer from $\{u, u^*\}$ back to $\{u, u^*\}$

which proves condition Eq. (32) of Lemma 6. It remains to check condition Eq. (33). Using Eq. (68) again one gets

$$\begin{aligned} \langle S' | (V_{\text{main}})_{-+} H_0^{-1} (V_{\text{main}})_{+-} | S \rangle &= t^{2/3} \sum_{u \in S} d(u) \delta_{S, S'} = \langle S' | t^{2/3} \sum_{u \in U} d(u) n_u | S \rangle \\ &= \langle S' | \tilde{V}_{\text{extra}} | S \rangle. \end{aligned} \quad (71)$$

Here $(V_{\text{main}})_{+-}$ moves a particle from u^* to $u+v$ and $(V_{\text{main}})_{-+}$ returns the particle back from $u+v$ to u^* . Thus all conditions of Lemma 6 are satisfied.

Suppose now that $H_{\text{target}} \in \text{HCB}_2(n, m, J)$ has non-homogeneous hopping amplitudes, that is,

$$H_{\text{target}} = - \sum_{(u,v) \in E} t_{u,v} W_{u,v} + H_{\text{diag}}, \quad 0 \leq t_{u,v} \leq t. \quad (72)$$

By definition, $t \leq J$. Let (η, ϵ) be the desired simulation error, see Definition 1. Since we only need to approximate H_{target} with an error $\epsilon/2$, see Lemma 6, we can assume that

$$\frac{\epsilon}{2|E|} \leq t_{u,v} \leq t \quad \text{for all } (u, v) \in E.$$

For each node $w = u + v \in U^+$ define

$$\Delta_w = \sqrt{\frac{t}{t_{u,v}}}.$$

Note that $1 \leq \Delta_w \leq \sqrt{2J\epsilon^{-1}|E|} \leq \text{poly}(n, J, \epsilon^{-1})$. Given a node $u \in U$, let $\mathcal{N}(u) \subseteq U$ be the set of all nearest neighbors of u in the graph G . Define

$$d(u) = t^{-1/2} \sum_{v \in \mathcal{N}(u)} \sqrt{t_{u,v}} \quad \text{and} \quad d_2(u) = t^{-1} \sum_{v \neq v' \in \mathcal{N}(u)} \sqrt{t_{u,v} t_{u,v'}}.$$

Let H_{sim} be the HCD simulator defined by Eqs. (64–67). Exactly the same arguments as above show that H_{sim} satisfies conditions of Lemma 6 with the target Hamiltonian Eq. (72).

We conclude that any Hamiltonian $H_{\text{target}} \in \text{HCB}_2(n, m, J)$ can be simulated with an error (η, ϵ) by a Hamiltonian $H_{\text{sim}} \in \text{HCD}(n', m, J')$ where $n' = O(n^2)$ and $J' = \text{poly}(n, J, \epsilon^{-1}, \eta^{-1})$. The simulation uses an encoding \mathcal{E} that represents each particle of the target model by a dimer in the simulator model. In particular, \mathcal{E} maps basis vectors to basis vectors. Note that the extended graph G' is triangle-free regardless of the original graph G , so the reduction from TIM to HCD described in Sect. 6 and the reduction from HCD to range-2 HCB can be composed.

8. Range-2 Bosons with Multi-particle Interactions

In this section we describe a second-order reduction that uses range-2 HCB as a simulator and generates the same range-2 HCB Hamiltonian but with certain additional multi-particle interactions. This reduction is only needed for the proof of Theorem 2.

Consider a graph $G = (U, E)$. For any subset of nodes $S \subseteq U$ define a diagonal operator

$$D(S) = \prod_{u \in S} (I - n_u).$$

Let $d \leq \text{poly}(n)$ be any integer and $S_1, \dots, S_d \subseteq U$ be arbitrary subsets of nodes. Suppose our target Hamiltonian is

$$H_{\text{target}} = H_{\text{bos}} - \sum_{\alpha=1}^d p_{\alpha} D(S_{\alpha}). \quad (73)$$

Here $H_{\text{bos}} \in \text{HCB}_2(n, m, J)$ describes the range-2 HCB on the graph G and $0 \leq p_{\alpha} \leq J$ are arbitrary coefficients. The Hamiltonian H_{target} acts on the m -particle sector $\mathcal{B}_m(G)$. Let us show how to simulate H_{target} using the standard range-2 HCB model. The simulator will be defined on an extended graph $G' = (U', E')$ obtained from G by adding extra nodes and extra edges. For each interaction $D(S_{\alpha})$ in Eq. (73) let us add two extra nodes denoted $a(\alpha)$ and $b(\alpha)$. We connect the node $b(\alpha)$ by an edge with every node $u \in S_{\alpha}$. In addition, we connect the nodes $a(\alpha)$ and $b(\alpha)$ with each other, see Fig. 6. The number of particles in the simulator model is $m' = m + d$, where d is the number of extra terms in Eq. (73). Define a simulator Hamiltonian as

$$H_{\text{sim}} = \Delta H_0 + V, \quad H_0 = \sum_{\alpha=1}^d I - n_{a(\alpha)}, \quad V = \Delta^{1/2} V_{\text{main}} + V_{\text{extra}}, \quad (74)$$

$$V_{\text{main}} = - \sum_{\alpha=1}^d \sqrt{p_{\alpha}} W_{a(\alpha), b(\alpha)} \quad \text{and} \quad V_{\text{extra}} = H_{\text{bos}}. \quad (75)$$

Clearly, H_0 has zero ground state energy and the ground subspace of H_0 is spanned by all 2-sparse configurations of particles in G' such that the node $a(\alpha)$ is occupied for each α . Note that the node $b(\alpha)$ must be empty due to the 2-sparsity constraint. Define an encoding $\mathcal{E} : \mathcal{B}_m(G) \rightarrow \mathcal{B}_{m+d}(G')$ as follows. If $S \subseteq U$ is a 2-sparse subset,

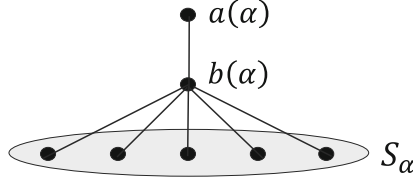


Fig. 6. Simulation of multi-particle interactions $D(S_\alpha)$. We choose $H_0 = I - n_{a(\alpha)}$ such that the node $a(\alpha)$ is occupied for any ground state of H_0 . Then the node $b(\alpha)$ must be empty due to the 2-sparsity constraint. The perturbation V moves the particle from $a(\alpha)$ to $b(\alpha)$ or vice versa

define $\mathcal{E}(S) = S \cup \{a(1), \dots, a(d)\} \subseteq U'$. Note that $\mathcal{E}(S)$ is a 2-sparse subset since a node $a(\alpha)$ has only one neighbor $b(\alpha)$ and the latter never belongs to $\mathcal{E}(S)$. Define $\mathcal{E}|S\rangle = |\mathcal{E}(S)\rangle$. The above shows that \mathcal{E} is an isometry and the image of \mathcal{E} coincides with the ground subspace of H_0 . Let us check that the perturbation V satisfies conditions of Lemma 5. Obviously, $(V_{\text{main}})_{--} = 0$ since any term in V_{main} moves a particle from $a(\alpha)$ to $b(\alpha)$ or vice versa. The operator V_{extra} is block-diagonal since it acts trivially on the extra nodes $a(\alpha), b(\alpha)$. Let us check condition Eq. (31) of Lemma 5. Note that no hopping in the original graph G is prohibited due to the presence of extra particles at $a(\alpha)$ since these particles are separated from any node of G by at least two edges. Thus $(V_{\text{extra}})_{--} = \overline{H_{bos}}$, where $\overline{H_{bos}} = \mathcal{E}H_{bos}\mathcal{E}^\dagger$ is the encoded version of H_{bos} . Let us compute $(V_{\text{main}})_{-+}H_0^{-1}(V_{\text{main}})_{+-}$. Suppose $|S\rangle$ is a ground state of H_0 . The 2-sparsity condition implies that a node $b(\alpha)$ cannot be occupied if S_α contains at least one particle. This shows that $(W_{a(\alpha),b(\alpha)})_{+-}|S\rangle = 0$ if $S \cap S_\alpha \neq \emptyset$, otherwise, $(W_{a(\alpha),b(\alpha)})_{+-}$ moves the particle from $a(\alpha)$ to $b(\alpha)$. Thus

$$(W_{a(\alpha),b(\alpha)})_{+-}|S\rangle = D(S_\alpha)|S \setminus a(\alpha) \cup b(\alpha)\rangle.$$

Note that the state in the righthand side is an eigenvector of H_0 with an eigenvalue 1. Note also that if $(V_{\text{main}})_{+-}$ moves a particle from some node $a(\alpha)$ to $b(\alpha)$ then $(V_{\text{main}})_{-+}$ must return the particle from $b(\alpha)$ to $a(\alpha)$. Thus

$$(V_{\text{main}})_{-+}H_0^{-1}(V_{\text{main}})_{+-} = \sum_{\alpha=1}^r p_\alpha (W_{a(\alpha),b(\alpha)})_{-+}(W_{a(\alpha),b(\alpha)})_{+-} = \sum_{\alpha=1}^r p_\alpha \overline{D(S_\alpha)}.$$

Here we noted that $D(S_\alpha)^2 = D(S_\alpha) = \overline{D(S_\alpha)}$. Thus

$$(V_{\text{extra}})_{--} - (V_{\text{main}})_{-+}H_0^{-1}(V_{\text{main}})_{+-} = \overline{H_{bos}} - \sum_{\alpha=1}^r p_\alpha \overline{D(S_\alpha)} = \overline{H_{\text{target}}},$$

that is, all conditions of Lemma 5 are satisfied.

We have proved that any Hamiltonian $H_{\text{target}} \in \text{HCB}_2(n, m, J)$ with d extra diagonal terms $-p_\alpha D(S_\alpha)$ such that $0 \leq p_\alpha \leq J$ can be simulated with an error (η, ϵ) by the Hamiltonian $H_{\text{sim}} \in \text{HCB}_2(n', m', J')$, where $n' = n + 2d$, $m' = m + d$, and $J' = \text{poly}(n, J, \epsilon^{-1}, \eta^{-1})$. The simulation uses an encoding \mathcal{E} that maps basis vectors to basis vectors. We shall absorb the extra diagonal terms into the Hamiltonian H_{diag} in all subsequent reductions.

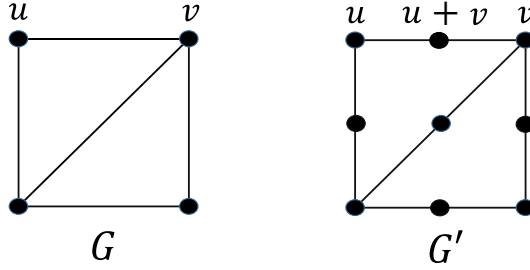


Fig. 7. Construction of the extended graph $G' = (U', E')$ for the range-2 HCB simulator starting from the graph $G = (U, E)$ for the target range-1 HCB

9. Reduction from Range-2 Bosons to Range-1 Bosons

In this section we construct a range-2 HCB simulator for a range-1 HCB model. It involves a second-order reduction. Consider a target Hamiltonian $H_{\text{target}} \in \text{HCB}(n, m, J)$ describing the m -particle sector of range-1 hard-core bosons on some graph $G = (U, E)$ with n nodes,

$$H_{\text{target}} = - \sum_{(u,v) \in E} t_{u,v} W_{u,v} + H_{\text{diag}}. \quad (76)$$

The range-2 HCB simulator will be defined on an extended graph $G' = (U', E')$ obtained from G by placing an extra node at the center of every edge of G , see Fig. 7 for an example. The extra node located at the center of an edge $(u, v) \in E$ will be denoted $u + v$. Then the extended graph G' has a set of nodes

$$U' = U \cup U^+, \quad U^+ = \{u + v : (u, v) \in E\}. \quad (77)$$

The simulator and the target models have the same number of particles m . Thus the simulator has Hilbert space $\mathcal{B}_{m,2}(G')$ spanned by 2-sparse m -node subsets in the graph G' . Define a simulator Hamiltonian as $H_{\text{sim}} = \Delta H_0 + V$, where

$$H_0 = \sum_{w \in U^+} n_w \quad (78)$$

penalizes particles that occupy nodes located at the centers of edges of G . We choose the perturbation as $V = \Delta^{1/2} V_{\text{main}} + V_{\text{extra}}$, where

$$V_{\text{main}} = - \sum_{(u,v) \in E'} t_{u,v}^{1/2} W_{u,v}, \quad (79)$$

$$V_{\text{extra}} = H_{\text{diag}} + \sum_{(u,v) \in E} t_{u,v} (n_u - n_v)^2. \quad (80)$$

The sum in V_{extra} runs over pairs of nodes $u, v \in U$ considered as nodes of G' . Clearly, H_0 has zero ground state energy and its ground subspace is spanned by subsets of nodes $S \subseteq U'$ such that $S \cap U^+ = \emptyset$ and $|S| = m$. Note that any distinct nodes of S are automatically separated by at least two edges of G' , that is, S is a 2-sparse

subset. Given any subset of nodes $S \subseteq U$ in the graph G such that $|S| = m$, let $\mathcal{E}(S)$ be the corresponding subset of nodes in the graph G' . We define the encoding $\mathcal{E} : \mathcal{B}_m(G) \rightarrow \mathcal{B}_{m,2}(G')$ such that $\mathcal{E}|S\rangle = |\mathcal{E}(S)\rangle$. The above shows that $\text{Im}(\mathcal{E})$ coincides with the ground subspace of H_0 .

Let us check that the perturbation V satisfies the conditions of Lemma 5. First, we note that $(V_{\text{main}})_{--} = 0$. Indeed, suppose $S \subseteq U'$ is a ground state of H_0 . Then $S \cap U^+ = \emptyset$. Thus V_{main} can only move a particle from some node $u \in U$ to some node $v \in U^+$ which produces an excited state of H_0 . The operator V_{extra} is block diagonal because it is diagonal.

Let us now check condition Eq. (31) of Lemma 5. Consider any ground state of H_0 , that is, m -node subset $S \subseteq U'$ such that $S \cap U^+ = \emptyset$. We claim that

$$(V_{\text{main}})_{+-}|S\rangle = - \sum_{u \in S} \sum_{(u,v) \in E} t_{u,v}^{1/2} (1 - n_v) W_{u,u+v} |S\rangle. \quad (81)$$

Indeed, the hopping terms in V_{main} can only move a particle from some node $u \in S$ to some node $u + v$ such that $(u, v) \in E$ and such that the resulting configuration of particles is 2-sparse. The latter condition is satisfied iff $n_v = 0$. Taking into account that $W_{u,u+v}|S\rangle$ is an eigenvector of H_0^{-1} with an eigenvalue one, we get

$$(V_{\text{main}})_{-+} H_0^{-1} (V_{\text{main}})_{+-} = \sum_{(u,v) \in E} t_{u,v} W_{u,v} + \sum_{u \in U} \sum_{(u,v) \in E} t_{u,v} n_u (1 - n_v). \quad (82)$$

Here the last term accounts for double-hopping processes where $(V_{\text{main}})_{+-}$ moves a particle from u to $u + v$ and $(V_{\text{main}})_{-+}$ returns the particle back to u . Using the identity $n_u(1 - n_v) + n_v(1 - n_u) = (n_u - n_v)^2$ one gets

$$(V_{\text{main}})_{-+} H_0^{-1} (V_{\text{main}})_{+-} = \sum_{(u,v) \in E} t_{u,v} W_{u,v} + \sum_{(u,v) \in E} t_{u,v} (n_u - n_v)^2. \quad (83)$$

The last term is exactly cancelled by V_{extra} which proves condition Eq. (31) of Lemma 5. Note that in this case the logical operators $\overline{W}_{u,v}$ and \overline{n}_u coincide with $W_{u,v}$ and n_u since we encode each particle of the target model by a single particle in the simulator model.

To conclude, we have proved that any Hamiltonian $H_{\text{target}} \in \text{HCB}(n, m, J)$ can be simulated with an error (η, ϵ) by the Hamiltonian $H_{\text{sim}} \in \text{HCB}_2(n', m, J')$, where $n' = O(n^2)$ and $J' = \text{poly}(n, J, \epsilon^{-1}, \eta^{-1})$. The simulation uses an encoding \mathcal{E} that maps basis vectors to basis vectors.

10. Range-1 Bosons with a Controlled Hopping

Consider a graph $G = (U, E)$ with n nodes and a Hamiltonian $H_{\text{bos}} \in \text{HCB}(n, m, J)$ describing the m -particle sector of the range-1 HCB model on the graph G . Suppose our target Hamiltonian is

$$H_{\text{target}} = H_{\text{bos}} - \sum_{(c;u,v)} t_{c;u,v} n_c W_{u,v}, \quad (84)$$

where the sum runs over all triples of nodes $(c; u, v)$ such that $c \in U$, $(u, v) \in E$, and $c \notin \{u, v\}$. The term $n_c W_{u,v}$ describes a controlled hopping process where the presence of particle at the node c controls whether the hopping between nodes u, v is turned on

or off. The coefficients $t_{c;u,v}$ are the controlled hopping amplitudes. We shall always assume that $t_{c;u,v} \geq 0$. The Hamiltonian H_{target} acts on the m -particle sector $\mathcal{B}_m(G)$. Let $\text{HCB}^*(n, m, J)$ be the set of Hamiltonians H_{target} defined above where $0 \leq t_{c;u,v} \leq J$. In this section we show how to simulate H_{target} by the standard range-1 HCB. The simulation involves a composition of a first-order and a second-order reduction.

The simulator model will be defined on a graph $G' = (U', E')$ obtained from G by adding certain extra nodes and extra edges. Namely, for each triple $(c; u, v)$ that appears in Eq. (84) we add an extra node $a(c; u, v)$ and a pair of extra edges connecting $a(c; u, v)$ to u and v . Let $n' = |U'|$ be the number of nodes in the extended graph and $U^+ \subseteq U'$ be the set of all extra nodes $a(c; u, v)$. The simulator and the target models have the same number of particles m .

Our first reduction has a simulator Hamiltonian

$$\tilde{H}_{\text{sim}} = \tilde{\Delta} \tilde{H}_0 + \tilde{V}, \quad \tilde{H}_0 = \sum_{(c;u,v)} (I - n_c) n_{a(c;u,v)}, \quad (85)$$

where $\tilde{V} \in \text{HCB}(n', m, \tilde{J})$ will be chosen at the next reduction. The Hamiltonian \tilde{H}_{sim} acts on the Hilbert space $\mathcal{B}_m(G')$. Let $\tilde{\mathcal{H}}_-$ be the ground subspace of \tilde{H}_0 . Obviously, $\tilde{\mathcal{H}}_-$ is spanned by configurations of particles such that a node $a(c; u, v)$ can be occupied only if c is occupied. This property must hold for each extra node $a(c; u, v)$. Lemma 4 shows that \tilde{H}_{sim} can simulate the restriction of any Hamiltonian from $\text{HCB}(n', m, \tilde{J})$ onto the subspace $\tilde{\mathcal{H}}_-$. In the rest of this section we assume that our full Hilbert space is $\mathcal{H} = \tilde{\mathcal{H}}_-$. The above simulation uses the trivial encoding, that is, $\mathcal{E}|S\rangle = |S\rangle$ if $S \subseteq U^+$ is a ground state of \tilde{H}_0 and $\mathcal{E}|S\rangle = 0$ otherwise.

Our second reduction has a simulator Hamiltonian

$$H_{\text{sim}} = \Delta H_0 + V, \quad H_0 = \Delta \sum_{a \in U^+} n_a, \quad V = \Delta^{1/2} V_{\text{main}} + V_{\text{extra}}, \quad (86)$$

where

$$V_{\text{main}} = - \sum_{(c;u,v)} (t_{c;u,v})^{1/2} (W_{u,a(c;u,v)} + W_{v,a(c;u,v)}), \quad (87)$$

$$V_{\text{extra}} = H_{\text{bos}} + \sum_{(c;u,v)} t_{c;u,v} n_c (n_u + n_v). \quad (88)$$

Here all operators are restricted to the subspace \mathcal{H} defined above. We choose an encoding $\mathcal{E} : \mathcal{B}_m(G) \rightarrow \mathcal{H}$ that maps subsets of nodes in the graph G to the corresponding subsets of nodes in the extended graph G' . Obviously, $S \subseteq U^+$ is a ground state of H_0 iff $|S| = m$ and $S \cap U^+ = \emptyset$, that is, all the extra nodes $a(c; u, v)$ are empty. Thus $\text{Im}(\mathcal{E})$ coincides with the ground subspace of H_0 .

Let us check that the perturbation V satisfies all conditions of Lemma 5. We note that $(V_{\text{main}})_{--} = 0$ since V_{main} can only move a particle from (to) some ancillary node $a(c; u, v)$ which must be empty in any ground state of H_0 . The Hamiltonian V_{extra} is block-diagonal since H_{bos} acts trivially on all ancillary nodes whereas the second term in V_{extra} is diagonal. It remains to check condition Eq. (31) of Lemma 5. Let $S \subseteq U^+$ be any ground state of H_0 . Then $S \cap U^+ = \emptyset$. We claim that $W_{u,a(c;u,v)}|S\rangle = 0$ unless $n_c = 1$. Indeed, if $n_c = 0$ and $n_u = 0$ then both nodes u and $a(c; u, v)$ are empty. If $n_c = 0$ and $n_u = 1$ then $W_{u,a(c;u,v)}$ moves a particle from u to $a(c; u, v)$. However, a state in which the node $a(c; u, v)$ is occupied and the node c is empty is orthogonal to the

subspace \mathcal{H} . Since the simulator model is restricted to \mathcal{H} , we have $W_{u,a(c;u,v)}|S\rangle = 0$ in both cases. In the remaining case, $n_c = 1$, one has $W_{u,a(c;u,v)}|S\rangle = |S'\rangle$, where $S' = (S \setminus u) \cup a(c; u, v)$. The above shows that

$$(V_{\text{main}})_{-+} H_0^{-1} (V_{\text{main}})_{+-} = \sum_{(c;u,v)} t_{c;u,v} n_c (W_{u,v} + n_u + n_v). \quad (89)$$

Here the first term describes processes where $(V_{\text{main}})_{+-}$ moves a particle from u to $a(c; u, v)$ and $(V_{\text{main}})_{-+}$ moves the particle from $a(c; u, v)$ to v . The last two terms describe processes where $(V_{\text{main}})_{+-}$ moves a particle from u to $a(c; u, v)$ and $(V_{\text{main}})_{-+}$ returns the particle back to u . The last two terms in Eq. (89) are canceled by V_{extra} . This proves condition Eq. (31) of Lemma 5. Note that in this case the logical operators $\bar{W}_{u,v}$ and \bar{n}_u coincide with $W_{u,v}$ and n_u since we encode each particle of the target model by a single particle in the simulator model.

Combining Lemmas 3, 4 and 5 we conclude that any Hamiltonian $H_{\text{target}} \in \text{HCB}^*(n, m, J)$ can be simulated with an error (η, ϵ) by the Hamiltonian $\tilde{H}_{\text{sim}} \in \text{HCB}(n', m, J')$ where $n' = O(n^3)$ and $J' = \text{poly}(n, J, \epsilon^{-1}, \eta^{-1})$. The simulation uses an encoding \mathcal{E} that maps basis vectors to basis vectors.

11. From Range-1 Bosons to 2-Local Stoquastic Hamiltonians

Let us start from a simple classification of two-qubit stoquastic interactions. In this section we use the standard $|0\rangle, |1\rangle$ basis for a single qubit and the corresponding product basis for n qubits.

Lemma 9. *Let H be a two-qubit hermitian operator such that H has real matrix elements in the standard basis and all off-diagonal matrix elements of H are non-positive. Then H can be written as a sum of some diagonal two-qubit Hamiltonian H_{diag} and a convex linear combination of operators*

1. $-X \otimes |0\rangle\langle 0|$ and $-X \otimes |1\rangle\langle 1|$
2. $-|0\rangle\langle 0| \otimes X$ and $-|1\rangle\langle 1| \otimes X$
3. $-X \otimes X - Y \otimes Y$
4. $-X \otimes X + Y \otimes Y$

Proof. Let $G \equiv -H$. Since G has real matrix elements, the expansion of G in the basis of Pauli operators contains only the terms with even number of Y 's. Thus

$$G = -H_{\text{diag}} + h_{XI} X \otimes I + h_{IX} I \otimes X + h_{XX} X \otimes X + h_{XZ} X \otimes Z + h_{ZZ} Z \otimes X + h_{YY} Y \otimes Y, \quad (90)$$

where H_{diag} is some diagonal Hamiltonian. From

$$\langle 0, 0|G|1, 1\rangle = h_{XX} - h_{YY} \geq 0 \quad \text{and} \quad \langle 0, 1|G|1, 0\rangle = h_{XX} + h_{YY} \geq 0$$

one gets

$$h_{XX} X \otimes X + h_{YY} Y \otimes Y = p(X \otimes X + Y \otimes Y) + q(X \otimes X - Y \otimes Y), \quad (91)$$

where $p = (h_{XX} + h_{YY})/2$ and $q = (h_{XX} - h_{YY})/2$ are non-negative coefficients. From

$$\langle 0, 0|G|1, 0\rangle = h_{XI} + h_{XZ} \geq 0 \quad \text{and} \quad \langle 0, 1|G|1, 1\rangle = h_{XI} - h_{XZ} \geq 0$$

one gets

$$h_{XI}X \otimes I + h_{XZ}X \otimes Z = pX \otimes |0\rangle\langle 0| + qX \otimes |1\rangle\langle 1|, \quad (92)$$

where $p = h_{XI} + h_{XZ}$ and $q = h_{XI} - h_{XZ}$ are non-negative coefficients. Similar calculation shows that

$$h_{IX}I \otimes X + h_{ZX}Z \otimes X = p|0\rangle\langle 0| \otimes X + q|1\rangle\langle 1| \otimes X, \quad (93)$$

where $p = h_{IX} + h_{ZX}$ and $q = h_{IX} - h_{ZX}$ are non-negative coefficients. The lemma now follows from Eqs. (90–93). \square

Let $H_{\text{target}} \in \text{StoQLH}(n, J)$ be some fixed 2-local stoquastic Hamiltonian on n qubits. Our goal is to simulate H_{target} by some Hamiltonian $H_{\text{sim}} \in \text{HCB}^*(n', m, J')$. Recall that the latter describes the m -particle sector of range-1 hard-core bosons with a controlled hopping on some graph $G = (U, E)$ with n' nodes, see Sect. 10. We shall represent the j -th qubit of the target model by a pair of nodes $\{2j - 1, 2j\} \subseteq U$. The two basis states $|0\rangle$ and $|1\rangle$ of the j -th qubit are represented by a particle located at the node $2j - 1$ and $2j$ respectively (the dual rail representation). Thus the number of particles in the simulator model is $m = n$.

For the sake of clarity we shall first explain how to construct an HCB^* simulator individually for each two-qubit stoquastic interaction listed in Lemma 9. Thus we shall first consider the case $n = m = 2$. We shall simulate interactions (1) and (2) using a first-order reduction. Interactions (3) and (4) will require a composition of a first-order and a third-order reductions. Then we shall explain how to combine the simulators together. To avoid interference between simulators we shall introduce some ancillary nodes such that a simulator is activated only if the corresponding ancillary node is occupied by a particle.

Consider first the case $H_{\text{target}} = -pX \otimes |0\rangle\langle 0|$ with $p > 0$. The HCB^* simulator is defined on a graph $G = (U, E)$, where $U = \{1, 2, 3, 4\}$ and $E = \{1, 2\}$. The total number of particles is $m = 2$, so that the simulator Hilbert space is $\mathcal{B}_2(G)$. The simulator Hamiltonian is chosen as

$$H_{\text{sim}} = \Delta H_0 + V, \quad H_0 = n_1 n_2 + n_3 n_4, \quad (94)$$

$$V = -pn_3 W_{1,2}. \quad (95)$$

Ground states of H_0 are subsets of nodes $\{i, j\} \subseteq U$, where $i \in \{1, 2\}$ and $j \in \{3, 4\}$. The ground subspace of H_0 encodes two logical qubits as follows:

$$|\overline{0}, \overline{0}\rangle = |1, 3\rangle, \quad |\overline{0}, \overline{1}\rangle = |1, 4\rangle, \quad |\overline{1}, \overline{0}\rangle = |2, 3\rangle, \quad |\overline{1}, \overline{1}\rangle = |2, 4\rangle. \quad (96)$$

This is analogous to applying the dual-rail representation to each qubit. Obviously, V commutes with H_0 . Note that $W_{1,2}$ implements the logical \overline{X} on the first qubit and n_3 implements the logical operator $|\overline{0}\rangle\langle \overline{0}|$ on the second qubit. Lemma 4 implies that H_{sim} can simulate the restriction of V onto the logical subspace, that is, $V_{--} = -p\overline{X} \otimes |\overline{0}\rangle\langle \overline{0}|$. This is the desired target Hamiltonian. Using the same method one can simulate all elementary interactions (1) and (2) in Lemma 9.

Next consider the case

$$H_{\text{target}} = -(p/2)(X \otimes X + Y \otimes Y) = -p(|1, 0\rangle\langle 0, 1| + |0, 1\rangle\langle 1, 0|), \quad p > 0. \quad (97)$$

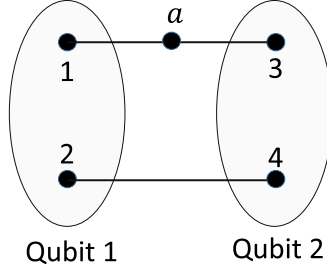


Fig. 8. Graph $G = (U, E)$ of the HCB^* simulator for the target Hamiltonian $-X \otimes X - Y \otimes Y$. The total number of particles is $m = 2$

The HCB^* simulator will be defined on a graph $G = (U, E)$ where $U = \{1, 2, 3, 4, a\}$, see Fig. 8. We choose the total number of particles $m = 2$. The simulation involves a composition of a first-order and a second-order reductions.

Our first reduction has a simulator Hamiltonian

$$\tilde{H}_{\text{sim}} = \tilde{\Delta} \tilde{H}_0 + \tilde{V}, \quad \tilde{H}_0 = n_1 n_2 + n_3 n_4, \quad \tilde{V} \in \text{HCB}^*(5, 2, \tilde{J}). \quad (98)$$

All above operators act on the Hilbert space $\mathcal{B}_2(G)$. The perturbation \tilde{V} will be chosen at the next reduction. Let \mathcal{H} be the ground subspace of \tilde{H}_0 . It is spanned by configurations of particles such that each qubit $\{1, 2\}$ and $\{3, 4\}$ contains at most one particle. Lemma 4 implies that \tilde{H}_{sim} can simulate the restriction of any HCB^* Hamiltonian \tilde{V} onto the subspace \mathcal{H} . Below we assume that our full Hilbert space is \mathcal{H} .

Our second reduction has a simulator Hamiltonian

$$H_{\text{sim}} = \Delta H_0 + V, \quad H_0 = n_a, \quad V = \Delta^{2/3} V_{\text{main}} + \Delta^{1/3} \tilde{V}_{\text{extra}}, \quad (99)$$

where

$$V_{\text{main}} = -p^{1/3} (W_{1,a} + W_{3,a} + n_a W_{2,4}), \quad (100)$$

$$\tilde{V}_{\text{extra}} = p^{2/3} (2n_1 n_3 + n_1 n_4 + n_2 n_3). \quad (101)$$

Here all operators are restricted to the subspace \mathcal{H} with at most one particle per qubit. Note that H_{sim} is an HCB^* Hamiltonian. The ground subspace of H_0 encodes two logical qubits according to Eq. (96). Let us check that the perturbation satisfies all conditions of Lemma 6. Note that $(V_{\text{main}})_{--} = 0$ since V_{main} can only move a particle from (to) the ancillary node a . The last term in V_{main} does not contribute to $(V_{\text{main}})_{--}$ since $n_a = 0$ for any ground state of H_0 . Obviously, \tilde{V}_{extra} is block-diagonal.

Let us check condition Eq. (32) of Lemma 6. Informally, it says that the third-order hopping process generated by V_{main} must implement the logical hopping operator between the two logical qubits. For example, suppose the initial state is $|\bar{0}, \bar{1}\rangle = |1, 4\rangle$. Then $(V_{\text{main}})_{+-}$ moves a particle from 1 to a by applying $W_{1,a}$, then $(V_{\text{main}})_{++}$ moves a particle from 4 to 2 by applying $n_a W_{2,4}$, and then $(V_{\text{main}})_{-+}$ moves a particle from a to 3 by applying $W_{3,a}$. This produces the correct final state $|\bar{1}, \bar{0}\rangle = |2, 3\rangle$. More formally, one can easily check that

$$\begin{aligned} (V_{\text{main}})_{+-} |\bar{1}, \bar{1}\rangle &= (V_{\text{main}})_{+-} |2, 4\rangle = 0, \\ (V_{\text{main}})_{+-} |\bar{0}, \bar{0}\rangle &= (V_{\text{main}})_{+-} |1, 3\rangle = -p^{1/3} (|3, a\rangle + |1, a\rangle), \\ (V_{\text{main}})_{+-} |\bar{0}, \bar{1}\rangle &= (V_{\text{main}})_{+-} |1, 4\rangle = -p^{1/3} |4, a\rangle, \\ (V_{\text{main}})_{+-} |\bar{1}, \bar{0}\rangle &= (V_{\text{main}})_{+-} |2, 3\rangle = -p^{1/3} |2, a\rangle. \end{aligned}$$

From this one easily gets

$$(V_{\text{main}})_{-+} H_0^{-1} (V_{\text{main}})_{++} H_0^{-1} (V_{\text{main}})_{+-} = -p |\overline{0}, \overline{1}\rangle \langle \overline{1}, \overline{0}| - p |\overline{1}, \overline{0}\rangle \langle \overline{0}, \overline{1}| = \overline{H}_{\text{target}}. \quad (102)$$

This proves condition Eq. (32). A similar calculation shows that

$$\begin{aligned} (V_{\text{main}})_{-+} H_0^{-1} (V_{\text{main}})_{+-} &= p^{2/3} (2|\overline{0}, \overline{0}\rangle \langle \overline{0}, \overline{0}| + |\overline{0}, \overline{1}\rangle \langle \overline{0}, \overline{1}| + |\overline{1}, \overline{0}\rangle \langle \overline{1}, \overline{0}|) \\ &= p^{2/3} (2n_1 n_3 + n_1 n_4 + n_2 n_3) \end{aligned} \quad (103)$$

which proves condition Eq. (33).

To compose the two reductions we extend H_{sim} defined in Eq. (99) to the full Hilbert space $\mathcal{B}_2(G)$ and substitute $\tilde{V} = H_{\text{sim}}$ into Eq. (98). Combining Lemmas 3, 4 and 6 we conclude that H_{target} can be simulated with an error (η, ϵ) by $\tilde{H}_{\text{sim}} \in \text{HCB}^*(5, 2, J')$ where $J' = \text{poly}(p, \eta^{-1}, \epsilon^{-1})$. The simulation uses the dual rail encoding \mathcal{E} defined in Eq. (96).

Finally, consider the case $H_{\text{target}} = -pX \otimes X + pY \otimes Y$, where $p > 0$. This Hamiltonian can be obtained from $H_{\text{target}} = -p(X \otimes X + Y \otimes Y)$ by conjugating the second qubit with X . This is equivalent to exchanging nodes 3 and 4 in the reduction described above. Hence we have constructed an HCB^* simulator for all elementary stoquastic interactions.

Suppose now that $H_{\text{target}} \in \text{StoqLH}(n, J)$ is a general 2-local stoquastic Hamiltonian on n qubits. By Lemma 9,

$$H_{\text{target}} = H_{\text{diag}} + \sum_{\alpha=1}^m p_{\alpha} H_{\alpha}, \quad (104)$$

where H_{diag} is a diagonal 2-local Hamiltonian with terms proportional to n_u and $n_u n_v$, where $p_{\alpha} > 0$ are some coefficients, and each term H_{α} is one of the four elementary stoquastic interactions applied to some pair of qubits. Obviously, the number of terms is $m \leq \text{poly}(n)$. The corresponding HCB^* simulator H_{sim} will be defined on a graph $G = (U, E)$ with $2n + m'$ nodes, where $m' \leq m$ is the number of interactions of type (3) or (4) in H_{target} , see Lemma 9. Without loss of generality, the first m' interactions H_{α} are of type (3) or (4). The total number of particles in the HCB^* simulator will be $m = n$, so that the Hilbert space of the simulator is $\mathcal{B}_n(G)$. We shall need a composition of a first-order and a third-order reductions.

Let us first define the set of nodes of G . Each qubit i gives rise to a pair of nodes $t(i)$ and $b(i)$ which form the dual-rail representation of the qubit. We encode the basis states $|0\rangle$ and $|1\rangle$ by a single particle located at the node $t(i)$ and $b(i)$ respectively. Each interaction H_{α} of type (3) or (4) gives rise to an extra node $a(\alpha)$ in G . This is the ancillary node used in the graph shown on Fig. 8.

The set of edges of G is defined as follows. For each interaction H_{α} of type (3) coupling qubits i, j we add an edge connecting nodes $t(i)$ and $a(\alpha)$, an edge connecting nodes $a(\alpha)$ and $t(j)$, and an edge connecting nodes $b(i)$ and $b(j)$. The last edge represents a controlled hopping with a control node $a(\alpha)$. For each interaction H_{β} of type (4) coupling qubits i, j we add an edge connecting nodes $t(i)$ and $a(\beta)$, an edge connecting nodes $a(\beta)$ and $b(j)$, and an edge connecting nodes $b(i)$ and $t(j)$. The last edge represents a controlled hopping with a control node $a(\beta)$. The resulting subgraph of G is shown on Fig. 9. This completes definition of the graph G for the HCB simulator.

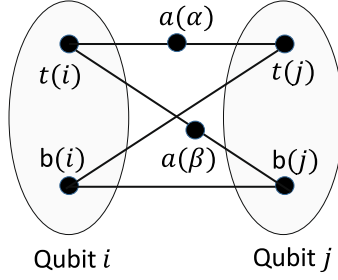


Fig. 9. Construction of the graph G for the HCB simulator. Each qubit i is represented by a pair of nodes $t(i), b(i)$ using the dual-rail representation. The ancillary node $a(\alpha)$ controls hopping between $b(i)$ and $b(j)$. The ancillary node $a(\beta)$ controls hopping between $b(i)$ and $t(j)$

Our first reduction has a simulator Hamiltonian

$$\tilde{H}_{\text{sim}} = \tilde{\Delta} \tilde{H}_0 + \tilde{V}, \quad \tilde{H}_0 = \sum_{i=1}^n n_{t(i)} n_{b(i)}, \quad \tilde{V} \in \text{HCB}^*(2n + m', n, \tilde{J}). \quad (105)$$

All above operators act on the Hilbert space $\mathcal{B}_n(G)$. The perturbation \tilde{V} will be chosen at the next reduction. Let \mathcal{H} be the ground subspace of \tilde{H}_0 . It is spanned by configurations of particles such that each qubit $\{t(i), b(i)\}$ contains at most one particle. Lemma 4 implies that \tilde{H}_{sim} can simulate the restriction of any HCB^* Hamiltonian \tilde{V} onto the subspace \mathcal{H} . Below we assume that our full Hilbert space is \mathcal{H} .

Our second reduction has a simulator Hamiltonian

$$H_{\text{sim}} = \Delta H_0 + V, \quad H_0 = \sum_{\alpha=1}^{m'} n_{a(\alpha)}, \quad V = \Delta^{2/3} V_{\text{main}} + \Delta^{1/3} \tilde{V}_{\text{extra}} + V_{\text{extra}}. \quad (106)$$

Since the total number of particles is n and each qubit may contain at most one particle, the ground subspace of H_0 is spanned by states with exactly one particle per qubit. It encodes n logical qubits under the dual rail representation. The perturbation operators are defined as the sums of respective perturbation operators over all individual simulators. More formally,

$$V_{\text{main}} = \sum_{\alpha=1}^{m'} V_{\text{main}}^{\alpha}, \quad \tilde{V}_{\text{extra}} = \sum_{\alpha=1}^{m'} \tilde{V}_{\text{extra}}^{\alpha}, \quad V_{\text{extra}} = H_{\text{diag}} + \sum_{\alpha=m'+1}^m V^{\alpha}, \quad (107)$$

where the perturbation operators carrying an index α are defined by Eqs. (95, 100, 101), depending on the type of the interaction H_{α} , with p replaced by p_{α} , with the nodes $\{1, 2\}$ replaced by the nodes of the first logical qubit acted upon by H_{α} , and with the nodes $\{3, 4\}$ replaced by the nodes of the second logical qubit acted upon by H_{α} .

Let us check that the perturbation V satisfies all conditions of Lemma 6. By definition, V_{extra} and \tilde{V}_{extra} act trivially on the ancillary nodes $a(\alpha)$ and thus they are block diagonal. Any term in V_{main} moves a particle to (from) some ancillary node $a(\alpha)$. Since all these nodes must be empty in the ground subspace of H_0 , one has $(V_{\text{main}})_{--} = 0$.

Let us now check condition Eq. (33). We claim that

$$(V_{\text{main}})_{-+} H_0^{-1} (V_{\text{main}})_{+-} = \sum_{\alpha=1}^{m'} (V_{\text{main}}^\alpha)_{-+} H_0^{-1} (V_{\text{main}}^\alpha)_{+-}. \quad (108)$$

Indeed, any term in $(V_{\text{main}})_{+-}$ must move a particle from some qubit node $u \in \{t(i), b(i)\}$ to some ancillary node $a(\alpha)$. In order to return the system to the ground subspace of H_0 , the factor $(V_{\text{main}})_{-+}$ must move the particle from $a(\alpha)$ to u . Thus $(V_{\text{main}}^\alpha)_{-+} H_0^{-1} (V_{\text{main}}^\beta)_{+-} = 0$ for $\alpha \neq \beta$. This implies Eq. (108). Since V_{main}^α and $\tilde{V}_{\text{extra}}^\alpha$ satisfy condition Eq. (33) for each individual simulator, Eq. (108) implies that V_{main} and \tilde{V}_{extra} also satisfy condition Eq. (33).

Next let us check condition Eq. (32) of Lemma 6. We claim that

$$(V_{\text{main}})_{-+} H_0^{-1} (V_{\text{main}})_{++} H_0^{-1} (V_{\text{main}})_{+-} = \sum_{\alpha=1}^m (V_{\text{main}}^\alpha)_{-+} H_0^{-1} (V_{\text{main}}^\alpha)_{++} H_0^{-1} (V_{\text{main}}^\alpha)_{+-} \quad (109)$$

Indeed, suppose $(V_{\text{main}})_{+-}$ moves a particle from a qubit node $u \in \{t(i), b(i)\}$ to some ancillary node $a(\alpha)$. For concreteness, assume that H_α is an interaction of type (3) coupling qubits i, j and $u = t(i)$. The factor $(V_{\text{main}})_{++}$ can either apply the controlled hopping term proportional to $n_{a(\alpha)} W_{b(i), b(j)}$ or move a particle from some other qubit node $v \in \{t(i'), b(i')\}$ to some ancillary node $a(\beta)$ with $\alpha \neq \beta$. In the latter case, however, we create two excited ancillary nodes so that $(V_{\text{main}})_{-+}$ will not be able to return the system back to the ground subspace of H_0 . In the former case $(V_{\text{main}})_{-+}$ can return the system to the ground subspace of H_0 only by moving the particle from $a(\alpha)$ to some node of qubit i or j . This proves Eq. (109). Since V_{main}^α satisfies condition Eq. (32) for each individual simulator with $V_{\text{extra}}^\alpha = 0$, Eq. (109) implies that

$$(V_{\text{main}})_{-+} H_0^{-1} (V_{\text{main}})_{++} H_0^{-1} (V_{\text{main}})_{+-} = \sum_{\alpha=1}^{m'} p_\alpha \overline{H}_\alpha. \quad (110)$$

Furthermore, one has $(V^\alpha)_{--} = p_\alpha \overline{H}_\alpha$ for interactions of type (1) and (2), that is, for $m' < \alpha \leq m$. Therefore

$$(V_{\text{extra}})_{--} = \overline{H}_{\text{diag}} + \sum_{\alpha=m'+1}^m p_\alpha \overline{H}_\alpha. \quad (111)$$

Combining this and Eq. (110) one arrives at

$$(V_{\text{extra}})_{--} + (V_{\text{main}})_{-+} H_0^{-1} (V_{\text{main}})_{++} H_0^{-1} (V_{\text{main}})_{+-} = \overline{H}_{\text{target}}. \quad (112)$$

Thus all conditions of Lemma 6 are satisfied.

To compose the two reductions we extend H_{sim} defined in Eq. (106) to the full Hilbert space $\mathcal{B}_n(G)$ and substitute $\tilde{V} = H_{\text{sim}}$ into Eq. (105). Combining Lemmas 3, 4, 6 we conclude that any Hamiltonian $H_{\text{target}} \in \text{StoqLH}(n, J)$ can be simulated with an error (η, ϵ) by the Hamiltonian $\tilde{H}_{\text{sim}} \in \text{HCB}^*(n', n, J')$ where $n' = 2n + m' = O(n^2)$ and $J' = \text{poly}(n, J, \epsilon^{-1}, \eta^{-1})$. The simulation uses the dual rail encoding \mathcal{E} that maps basis vectors to basis vectors.

Finally, let us extend the above reduction to $(2, k)$ -local stoquastic Hamiltonians. We have to modify the simulator model by adding multi-particle interactions as described in Sect. 8. More precisely, consider the target Hamiltonian defined in Eq. (104) and suppose the term H_{diag} contains k -qubit diagonal interactions with strength at most J . Such Hamiltonian can be written as

$$H_{\text{diag}} = - \sum_{x \in \{0,1\}^k} \sum_{M \subseteq [n]} p(x, M) |x\rangle\langle x|_M, \quad (113)$$

where $p(x, M)$ are some real coefficients such that $|p(x, M)| \leq \text{poly}(J, n)$, and $|x\rangle\langle x|_M$ is the k -qubit projector $|x\rangle\langle x|$ acting on a subset of qubits M . Performing an overall energy shift one can achieve $p(x, M) \geq 0$ for all x and M . Consider any fixed projector $|x\rangle\langle x|_M$. Recall that the basis states $|0\rangle$ and $|1\rangle$ of the i -th qubit of the target model are encoded by a particle located at the node $t(i)$ and $b(i)$ respectively. It follows that the encoded version of a projector $|0\rangle\langle 0|_i$ can be written as $I - n_{b(i)}$. Likewise, the encoded version of a projector $|1\rangle\langle 1|_i$ can be written as $I - n_{t(i)}$. Thus the encoded version of the projector $|x\rangle\langle x|_M$ is

$$\overline{|x\rangle\langle x|}_M = \prod_{i \in M : x(i)=0} (I - n_{b(i)}) \prod_{i \in M : x(i)=1} (I - n_{t(i)}).$$

Here $x(i)$ denotes the bit of the string x associated with the i -th qubit. Let $S(x, M) \subseteq U$ be the union of all nodes $b(i)$ with $i \in M$ and $x(i) = 0$ and all nodes $t(i)$ with $i \in M$ and $x(i) = 1$. We conclude that the encoded version of H_{diag} is

$$\overline{H}_{\text{diag}} = - \sum_{x \in \{0,1\}^k} \sum_{M \subseteq [n]} p(x, M) \prod_{u \in S(x, M)} (I - n_u). \quad (114)$$

As we have shown in Sect. 8 any such Hamiltonian can be included into the range-2 HCB model by adding one extra second-order reduction. Thus all our results obtained for 2-local stoquastic Hamiltonians hold for $(2, k)$ -local stoquastic Hamiltonians.

12. Proof of the Main Theorems

Now we have all ingredients needed for the proof of Theorems 1 and 2. Consider a target Hamiltonian $H \in \text{StoQLH}(n, J)$ or $H \in \text{StoQLH}^*(n, J)$. Let us prove that H can be simulated with an arbitrarily small error (η, ϵ) , by a TIM Hamiltonian $H' \in \text{TIM}(n', J')$ such that $n' \leq \text{poly}(n)$ and $J' \leq \text{poly}(n, J, \epsilon^{-1}, \eta^{-1})$. Here we use the definition of simulation given in Sect. 3. The parameters η, ϵ will be specified later. Indeed, consider the sequence of perturbative reductions constructed in Sects. 5–11. It can be described by a sequence of Hamiltonians H_1, H_2, \dots, H_R and encodings $\mathcal{E}_1, \mathcal{E}_2, \dots, \mathcal{E}_{R-1}$ such that the Hamiltonian H_t and the encoding \mathcal{E}_t simulate H_{t+1} with a small error (η_t, ϵ_t) for each $t = 1, \dots, R-1$. Here $H_R = H$ is the desired target Hamiltonian and $H_1 = H'$ is a TIM Hamiltonian. Choose a simulation error $\eta_t = \eta/2R$ and $\epsilon_t = \epsilon/2R$ for each individual reduction. Since $R = O(1)$, this implies $\eta_t = \Omega(\eta)$ and $\epsilon_t = \Omega(\epsilon)$. By construction, each Hamiltonian H_t belongs to one of the classes defined in Table 2 with some number of nodes (qubits) n_t and some interaction strength J_t . In addition, each Hamiltonian H_t (except for H_R) is a sum of a strong unperturbed part $(H_t)_0$ with a

spectral gap $\Delta_t \gg \|H_{t+1}\|$ and a weak perturbation. We have shown that each reduction satisfies

$$n_t \leq \text{poly}(n_{t+1}) \quad \text{and} \quad J_t \leq \text{poly}(n_{t+1}, J_{t+1}, \epsilon^{-1}, \eta^{-1}) \quad (115)$$

where $t = 1, \dots, R-1$. Using the initial conditions $n_R = n$, $J_R = J$, and taking into account that $R = O(1)$, we conclude that $n' \equiv n_1 \leq \text{poly}(n)$ and $J' \equiv J_1 \leq \text{poly}(n, J, \epsilon^{-1}, \eta^{-1})$.

Let $\mathcal{E} = \mathcal{E}_1 \mathcal{E}_2 \cdots \mathcal{E}_{R-1}$ be the composition of all individual encodings. Applying Lemma 3 one infers that the Hamiltonian H_1 and the encoding \mathcal{E} simulate H_R with an error $(\tilde{\eta}, \tilde{\epsilon})$, where

$$\tilde{\eta} \leq \frac{\eta}{2} + O(\epsilon) \max_t \Delta_t^{-1} \quad \text{and} \quad \tilde{\epsilon} \leq \frac{\epsilon}{2} + O(\epsilon) \max_t \frac{\|H_{t+1}\|}{\Delta_t} \quad (116)$$

Increasing, if necessary, the spectral gaps Δ_t by a factor $\text{poly}(\eta^{-1})$ one can achieve $\tilde{\eta} \leq \eta$ and $\tilde{\epsilon} \leq \epsilon$.

To prove Theorem 1 we choose ϵ as the precision specified in the statement of the theorem. The parameter η does not play any role here. We have to use all reductions described in Sects. 5–11 except for the one of Sect. 8 (the latter generates multi-particle interactions that are only needed for the proof of Theorem 2). Then H_1 is a TIM Hamiltonian with interactions of degree-3. Lemma 1 implies that the i -th smallest eigenvalues of H_1 and H_R differ at most by ϵ for all $i = 1, \dots, 2^n$. This proves Theorem 1 with $H' = H_1$.

To prove Theorem 2 we shall choose $\epsilon \leq \delta/3$, where δ is the spectral gap of H . We have to use all reductions described in Sects. 6–11. By construction, the encodings \mathcal{E}_t used in all these reductions map basis vectors to basis vectors. In addition, one can efficiently compute the action of \mathcal{E}_t and \mathcal{E}_t^\dagger on any basis vector. Thus the same properties hold for the full encoding $\mathcal{E} = \mathcal{E}_1 \mathcal{E}_2 \cdots \mathcal{E}_{R-1}$. Lemma 1 implies that the Hamiltonian H_1 has a non-degenerate ground state and a spectral gap at least $\delta - 2\epsilon \geq \delta/3$. Let $|g\rangle$ and $|g'\rangle$ be the ground states of H and H_1 . By Lemma 2,

$$\| |g'\rangle - \mathcal{E}|g\rangle \| \leq \eta + C\delta^{-1}\epsilon$$

for some constant coefficient C . Choosing $\epsilon = \min(\delta/3, \eta\delta C^{-1})$ one can achieve $\| |g'\rangle - \mathcal{E}|g\rangle \| \leq 2\eta$. Since η can be arbitrarily small, this proves Theorem 2 with $H' = H_1$.

Let us remark that the map $H \rightarrow H'$ in Theorem 2 can be made sufficiently smooth. More precisely, suppose H smoothly depends on some parameter τ such that the j -th derivative of H with respect to τ has norm at most $\text{poly}(n)$ for any constant j . Then we claim that the j -th derivative of H' with respect to τ has norm at most $\text{poly}(n, \delta^{-1})$. Indeed, suppose $H_{\text{target}} = H_{t+1}$ and $H_{\text{sim}} = H_t$ are the target and the simulator Hamiltonians used in some individual reduction and (η_t, ϵ_t) is the desired simulation error. For concreteness, consider the reduction of Sect. 11. Note that the derivative of H_{sim} becomes infinite if some of the coefficients p_α in Eq. (104) becomes zero since H_{sim} contains terms proportional to $p_\alpha^{1/3}$ and $p_\alpha^{2/3}$. To avoid such singularities, let us choose a sufficiently small cutoff value p_{\min} and replace p_α by $\tilde{p}_\alpha = \sqrt{p_\alpha^2 + p_{\min}^2}$ in Eq. (104) (recall that the coefficients p_α must be non-negative). This gives a new target Hamiltonian $\tilde{H}_{\text{target}}$ such that $\|H_{\text{target}} - \tilde{H}_{\text{target}}\| \leq p_{\min} \text{poly}(n)$. We choose p_{\min} small enough so that $\|H_{\text{target}} - \tilde{H}_{\text{target}}\| \ll \epsilon_t$. Let \tilde{H}_{sim} be the simulator Hamiltonian constructed for

$\tilde{H}_{\text{target}}$. Then \tilde{H}_{sim} simulates H_{target} with the error approximately (η_t, ϵ_t) and the j -th derivative of \tilde{H}_{sim} has norm at most $\text{poly}(n, t_{\min}^{-1}) = \text{poly}(n, \epsilon_t^{-1}) = \text{poly}(n, \delta^{-1})$. By introducing a similar cutoff in all remaining reductions one can easily check that the j -th derivative of H' with respect to τ has norm at most $\text{poly}(n, \delta^{-1})$. It is known that an adiabatic path with the minimum spectral gap δ such that the j -th derivative has norm at most C_j can be traversed in time $T = O(C_1\delta^{-2} + C_2\delta^{-2} + C_1^2\delta^{-3})$, see [25]. This implies Corollary 4.

Finally, let us remark that Theorem 2 can be extended to TIM Hamiltonians with interactions of degree-3, although the corresponding encoding \mathcal{E} would no longer map basis vectors to basis vectors. Indeed, let us modify the above proof of Theorem 2 by including the reduction of Sect. 5. Then the final TIM Hamiltonian H' has interactions of degree-3. Let \mathcal{E}_1 be the encoding used in the reduction of Sect. 5. Recall that \mathcal{E}_1 encodes each qubit u of the target model into a one-dimensional chain L_u with a Hamiltonian $H_{\text{chain}} = -\sum_{j \in \mathbb{Z}_m} g Z_j Z_{j+1} + X_j$, where $m \leq \text{poly}(n)$ and $g \approx 1$, see Sect. 5. Basis states of the logical qubit are $|\bar{0}\rangle \sim |\psi_0\rangle + |\psi_1\rangle$ and $|\bar{1}\rangle \sim |\psi_0\rangle - |\psi_1\rangle$, where ψ_0 and ψ_1 are the ground states of H_{chain} satisfying $X^{\otimes m} \psi_{0,1} = \pm \psi_{0,1}$. Accordingly, the full encoding $\mathcal{E} = \mathcal{E}_1 \mathcal{E}_2 \cdots \mathcal{E}_{R-1}$ maps any basis vector to a tensor product of the states $|\bar{0}\rangle$ and $|\bar{1}\rangle$. Let us argue that the logical qubits can be efficiently initialized and measured. Choose any physical qubit $i \in L_u$. Using Eqs. (42, 43, 44) one gets $\langle \bar{0} | Z_i | \bar{0} \rangle = \xi$ and $\langle \bar{1} | Z_i | \bar{1} \rangle = -\xi$, where $\xi \geq \text{poly}(n^{-1})$. Thus one can measure the logical qubit u in the Z -basis by measuring any physical qubit of L_u in the Z -basis. However, the measurement has to be repeated $\text{poly}(n)$ times to get a reliable statistics. One can measure the logical qubit in the X -basis in a single shot by measuring every qubit of L_u in the X -basis. Computing the product of the measured outcomes gives the eigenvalue of $X^{\otimes m}$ which differentiates between ψ_0 and ψ_1 . Finally, the state $|\bar{\uparrow}\rangle = |\psi_0\rangle$ can be prepared by the adiabatic evolution starting from the product state $|+\rangle^{\otimes m}$ and adiabatically turning on the parameter g in the Hamiltonian H_{chain} . It is well-known that the minimum spectral gap of H_{chain} is $\Omega(m^{-1})$, so that the initialization can be done in time $\text{poly}(n)$. The logical state $|\bar{0}\rangle$ can be obtained from $|\bar{\uparrow}\rangle$ by adiabatically changing the logical Hamiltonian from $-\bar{X}$ to $-\bar{Z}$.

Acknowledgements. The authors would like to thank Barbara Terhal for helpful discussions on perturbative reductions. S.B. acknowledges NSF Grant CCF-1110941.

A. Bounds on the Energy Splitting and Matrix Elements for the Ising Chain

In this section we prove Eqs. (40, 44).

Let us first prove Eq. (40). Choose any $g^{-1} < R < 1$ and consider contours

$$C = \{z \in \mathbb{C}^2 : |z| = R\} \quad \text{and} \quad C^{-1} = \{z \in \mathbb{C}^2 : |z| = R^{-1}\}$$

We orient C and C^{-1} clockwise and counter-clockwise respectively. Denote $E_+ \equiv E_0$ and $E_- \equiv E_1$, see Fact 1. Using Eq. (37) one can easily check that

$$E_{\pm} = \frac{m}{2\pi i} \oint_{C_{UC^{-1}}} \frac{dz \sqrt{g^2 + 1 - g(z + z^{-1})}}{z(z^m \mp 1)}. \quad (117)$$

Since the contours C and C^{-1} can be mapped to each other via a change of variable $z \rightarrow z^{-1}$, one gets

$$E_{\pm} = -\frac{m}{2\pi i} \oint_C \frac{dz(1 \pm z^m)\sqrt{g^2 + 1 - g(z + z^{-1})}}{z(z^m \mp 1)}. \quad (118)$$

Therefore

$$\delta = E_- - E_+ = -\frac{2m}{\pi i} \oint_C \frac{dz z^{m-1} \sqrt{g^2 + 1 - g(z + z^{-1})}}{1 - z^{2m}}. \quad (119)$$

The function $\sqrt{g^2 + 1 - g(z + z^{-1})}$ is analytic in the complex plane with cuts along the intervals $[0, g^{-1}]$ and $[g, \infty]$. Deforming the contour C such that it goes from 0 to g^{-1} in the upper half-plane and then returns to 0 in the lower half-plane one gets

$$\delta = \frac{4m\sqrt{g}}{\pi} \int_0^{g^{-1}} \frac{x^{m-1} \sqrt{x + x^{-1} - g - g^{-1}} dx}{1 - x^{2m}}. \quad (120)$$

Using a bound

$$x + x^{-1} - g - g^{-1} = x^{-1}(g - x)(g^{-1} - x) \geq (g - g^{-1})x^{-1}(g^{-1} - x) \quad (121)$$

we obtain

$$\delta \geq \frac{4m\sqrt{g^2 - 1}}{\pi} \int_0^{g^{-1}} x^{m-3/2} \sqrt{g^{-1} - x} dx. \quad (122)$$

Making a change of variables $x = g^{-1}y$ one gets

$$\delta \geq \frac{4mg^{-m}\sqrt{g^2 - 1}}{\pi} \int_0^1 dy y^{m-3/2} \sqrt{1-y} \geq \Omega(1)g^{-m}m^{-1}\sqrt{g^2 - 1}. \quad (123)$$

Here we noted that the integral over y is equal to the beta function $B(m - 1/2, 3/2) = \Omega(m^{-2})$. Finally, since $\sqrt{g^2 - 1} = \Omega(m^{-1/2})$, one gets $\delta \geq \Omega(m^{-c-3/2})$. To get an upper bound in Eq. (40) we note that

$$x^{-1}(g - x)(g^{-1} - x) \leq gx^{-1}(g^{-1} - x) \quad \text{and} \quad (1 - x^{2m})^{-1} \leq (1 - g^{-2m})^{-1} \leq O(1).$$

Performing the same change of variable as above one gets

$$\begin{aligned} \delta &\leq O(mg^{-m+1}) \int_0^1 dy y^{m-3/2} \sqrt{1-y} = O(mg^{-m+1})B(m - 1/2, 3/2) \\ &= O(m^{-c-1/2}). \end{aligned} \quad (124)$$

Let us now prove Eq. (44). We shall use the notations of Fact 2. In the limit $g \rightarrow \infty$ the Hamiltonian Eq. (35) has ground states $|0^{\otimes m}\rangle$ and $|1^{\otimes m}\rangle$, that is,

$$|\psi_0\rangle = \frac{1}{\sqrt{2}}(|0^{\otimes m}\rangle + |1^{\otimes m}\rangle) \quad \text{and} \quad |\psi_1\rangle = \frac{1}{\sqrt{2}}(|0^{\otimes m}\rangle - |1^{\otimes m}\rangle).$$

Thus $\xi = \langle \psi_1 | Z_j | \psi_0 \rangle = 1$. Since ξ is a real continuous function of g , it suffices to show that $|\xi| \geq (1 - g^{-2})^{1/8}$ for all $g > 1$. Let us write $|\xi| = (1 - g^{-2})^{1/8}\eta$. Then we have

to prove that $\eta \geq 1$. Since we already know that $\eta = 1$ in the limit $g \rightarrow \infty$, it suffices to show that η is a monotone decreasing function of g for all $g > 1$. Below we prove that

$$\eta^{-1} \frac{\partial \eta}{\partial g} \leq 0 \quad \text{for all } g > 1. \quad (125)$$

Computing the derivative over g one gets

$$\dot{\epsilon}_p = \frac{1}{2} \left(\frac{g}{\epsilon_p} + \frac{\epsilon_p}{g} - \frac{1}{g\epsilon_p} \right)$$

and thus

$$\frac{\partial}{\partial g} \sum_p \sum_q \log(\epsilon_p + \epsilon_q) = \frac{m^2}{2g} + \frac{1}{2}(g - g^{-1}) \left(\sum_p \epsilon_p^{-1} \right) \left(\sum_q \epsilon_q^{-1} \right). \quad (126)$$

Here the sums over p and q can range over either \mathbb{Z}_m or $\mathbb{Z}_m + 1/2$. Using Eq. (126) one gets

$$\eta^{-1} \frac{\partial \eta}{\partial g} = \frac{1}{16}(g^{-1} - g)(Z_+ - Z_-)^2, \quad (127)$$

where

$$Z_+ \equiv \sum_{p \in \mathbb{Z}_m} \epsilon_p^{-1} \quad \text{and} \quad Z_- \equiv \sum_{q \in \mathbb{Z}_m + 1/2} \epsilon_q^{-1} \quad (128)$$

This implies Eq. (125) and proves that $\eta \geq 1$ for all $g > 1$.

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Communicated by M. M. Wolf