Simulation of Many-Body Hamiltonians using Perturbation Theory with Bounded-Strength Interactions

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We show how to map a given n-qubit target Hamiltonian with bounded-strength k-body interactions onto a simulator Hamiltonian with two-body interactions, such that the ground-state energy of the target and the simulator Hamiltonians are the same up to an extensive error $O(\epsilon n)$ for arbitrary small $\epsilon$. The strength of interactions in the simulator Hamiltonian depends on $\epsilon$ and $k$ but does not depend on $n$. We accomplish this reduction using a new way of deriving an effective low-energy Hamiltonian which relies on the Schrieffer-Wolff transformation of many-body physics.

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INTRODUCTION

In quantum field theory and quantum many-body physics perturbation theory is omnipresent. Perturbation theory is perhaps most important as a method for constructing an efficient description of the physics at low energies as an effective theory of the physics at higher energies. For systems which do not have a perturbative treatment, it can be much harder or impossible to obtain such a concise and efficient description. In an apparently independent development, perturbation theory has recently appeared as a tool in the area of quantum complexity theory [1]. Its use in this area resembles that in theoretical physics: it relates the low-energy properties of different Hamiltonian models. But in computer science this association is made in the reverse direction as compared with theoretical physics. In many-body physics, the “full” Hamiltonian (including high energy degrees of freedom) is given, and an effective Hamiltonian on the low-energy subspace is calculated using perturbation theory. In computational complexity theory, the effective Hamiltonian is given – it is a “target Hamiltonian” $H_{\text{target}}$ chosen for some computational hardness property (for example, in adiabatic quantum computation [2] the ground state of $H_{\text{target}}$ encodes the execution of a quantum algorithm). Then a “high-energy” simulator Hamiltonian $H$ is to be chosen such that $H_{\text{target}}$ can be obtained from it by perturbation theory. The main objective is to make the simulator Hamiltonian $H$ as simple and realistic as possible while retaining the computational hardness of $H_{\text{target}}$. For example, the perturbation theory has been used in [3] to prove universality of quantum adiabatic computation with local two-body Hamiltonians on a 2D square lattice. For more recent developments see [4, 5, 6, 7].

In all applications mentioned above, one deals with a many-body Hamiltonian $H = H_0 + V$ where $H_0$ is a simple operator with a known spectrum and $V$ is a perturbation. The spectrum of $H_0$ consists of two disjoint parts spanning the low-energy subspace $P$ and the high-energy subspace $Q$. The two parts of the spectrum are separated from each other by an energy gap $\Delta$. A perturbation expansion provides a systematic way of constructing an effective Hamiltonian $H_{\text{eff}}$ acting on the low-energy subspace $P$ such that the ground state energy of $H_{\text{eff}}$ approximates the one of $H$ with an arbitrarily small error. An important shortcoming of the perturbative approach is the limited range of parameters over which it can be rigorously justified, namely, $\|V\| < \Delta/2$, see for instance [1, 8]. For $\|V\| \gg \Delta$, we expect states from the high-energy subspace to mix strongly with states from the low-energy subspace. Thus, it should not be expected that a general perturbative expansion for $H_{\text{eff}}$ is convergent when $\|V\| \gg \Delta$. (One notable exception to this generic behavior is the case when the low-energy subspace is one-dimensional, see [3].)

If we require for convergence that $\|V\| \ll \Delta$, we force $\Delta$ to scale with system size $n$, since $\|V\|$ typically scales with $n$; this is what has been done in [1, 3, 4, 5, 6, 7]. Hence these calculations would indicate that perturbation theory can only be rigorously applied to an unphysical Hamiltonian, one for which the gap $\Delta$ grows with the system size $n$.

If the applicability of perturbation theory were thus limited, its common use in physics would be unwarranted. The lack of convergence of the perturbative series for quantum electrodynamics was argued on physical grounds by...
Dyson [10]. There is a widespread belief that general perturbative series for quantum field theory and many-body physics do not converge but are to be viewed as asymptotic series, meaning that their lowest-order terms are a good approximation to the quantity of interest (while inclusion of higher-order terms may actually give a worse result, see e.g. [8]).

In this Letter we make these beliefs more rigorous by developing a formalism that justifies application of perturbation theory in the regime \(||V|| \gg \Delta\). This formalism is applicable to many-body Hamiltonians that possess certain locality properties. A Hamiltonian \(H\) describing a system of \(n\) qubits will be called \(k\)-local if and only if it is represented as a sum of local interactions \(H = \sum_i H_i\) such that each operator \(H_i\) acts on some subset of \(k\) or less qubits. In addition, the Hamiltonians in this paper will have the important property that each qubit occurs in at most a constant, say \(m = O(1)\), number of terms \(H_i\). The constraint says that for growing system size, the number of interactions in which any one qubit participates does not grow, but stays constant. Such a condition is generically fulfilled for Hamiltonians with short-range interactions studied in physics. An example is the standard (2-local) Heisenberg Hamiltonian on a lattice \(H = -\sum_{i,j} J(rij)(X_iX_j + Y_iY_j + Z_iZ_j)\); the fact that the coupling \(J(rij)\) is bounded-range, \(J(rij > r) \approx 0\), ensures that each spin is acted upon by a constant number of terms. Note that our results are not restricted to Hamiltonians on lattices, but also hold for general networks of interactions such as expander graphs [11].

The interaction strength of a \(k\)-local Hamiltonian \(H = \sum_i H_i\) is defined as the largest norm of the local interactions, \(J = \max_i ||H_i||\). Throughout this paper we assume that \(k\) is a constant independent of \(n\).

Our main result is a rigorous bound on the error that is made when a perturbative expansion for the effective Hamiltonian is truncated at a low order (the second or the third) in the regime where the interaction strength of \(V\) is small compared to \(\Delta\) but \(||V|| \gg \Delta\). This bound allows us to prove the following result.

**Theorem 1.** Let \(H_{\text{target}}\) be a \(k\)-local Hamiltonian acting on \(n\) qubits with interaction strength \(J\). For any fixed precision \(\epsilon\) one can construct a 2-local simulator Hamiltonian \(H\) acting on \(O(n)\) qubits with interaction strength \(O(J)\) such that the ground state energy of \(H\) approximates the ground state energy of \(H_{\text{target}}\) with an absolute error at most \(\epsilon Jn\).

Let us comment on a significance of Theorem 1. First of all, it eliminates the essential shortcoming of the earlier constructions [1 2 3 4 5 6 7] mentioned above, namely, the unphysical scaling of the interaction strength in the simulator Hamiltonian \(H\). In our construction the interaction strength of \(H\) is bounded by a constant (depending only on \(k\), \(\epsilon\), and \(J\)) which makes it more physical and, in principle, implementable in a lab. The price we pay for this improvement is that we are able to reproduce the ground state energy only up to an extensive error \(\epsilon Jn\). For all realistic physical Hamiltonians the ground-state energy itself is generically proportional to \(nJ\), and thus the relative error can be made arbitrarily small. Secondly, estimating the ground-state energy of a \(k\)-local Hamiltonian up to some sufficiently small constant relative error is known to be an NP-hard problem even for classical (diagonal in the \(|0\rangle, |1\rangle\) basis) Hamiltonians. This hardness of approximation follows from the PCP theorem (PCP=probabilistically checkable proofs), see Chapter 29 of [11] for a review. Proving an analogous hardness of approximation result for quantum Hamiltonians is a widely anticipated development, a so called “quantum PCP theorem”, see Section 5 in [12]. If true, it would imply that reproducing the ground-state energy up to some sufficiently small relative error (which is what our simulation achieves) is enough to capture the computational hardness of the target Hamiltonian. We also believe that the simulation results reported in this Letter will be relevant in actually proving such a quantum PCP theorem. Finally, the techniques we develop may be relevant in the context of adiabatic quantum computation where the simulator Hamiltonian must be capable of reproducing ground-state expectation values of local observables, see [3, 13].

The proof of Theorem 1 relies on a new way of deriving an effective Hamiltonian, which we call the Schrieffer-Wolff transformation after its use in many-body physics [14]. Specifically, given an unperturbed Hamiltonian \(H_0\), projectors \(P, Q\) onto the low-energy and the high-energy subspaces of \(H_0\), and a perturbation \(V\), the Schrieffer-Wolff transformation is a unitary operator \(e^S\) with anti-hermitian \(S (S = -S^\dagger)\) such that (i) \(S\) is a block-off-diagonal operator, namely, \(PSP = 0\) and \(QSQ = 0\); (ii) the transformed Hamiltonian \(e^S(H_0 + V)e^{-S}\) is a block-diagonal operator, namely, \(Pe^S(H_0 + V)e^{-S}Q = 0\). Given such an operator \(S\), one defines the effective Hamiltonian on the low-energy subspace as \(H_{\text{eff}} = Pe^S(H_0 + V)e^{-S}P\). A detailed exposition of the Schrieffer-Wolff formalism will appear in [10].

Let us briefly sketch the proof of the theorem. The simulator Hamiltonian \(H\) is constructed using perturbation gadgets introduced in [1 2]. “Gadget” is a technical term used broadly in theoretical computer science; in the present application, a gadget is simply an extra mediator qubit, and a Hamiltonian coupling the mediator qubit with some small subset of system qubits. For every mediator qubit \(u\) we define a projector onto its low-energy subspace \(P_u^u = |0\rangle\langle 0|_u\) and its high-energy subspace \(Q_u^u = |1\rangle\langle 1|_u\). The purpose of a gadget is to simulate some particular \(k\)-body interaction
\( H_{\text{target}}^u \) in the decomposition \( H_{\text{target}} = \sum_u H_{\text{target}}^u + H_{\text{else}} \). Here \( H_{\text{else}} \) are additional terms in the target Hamiltonian that we do not wish to treat using perturbation theory (since they are already 2-local, for example).

Such simulation is achieved by applying perturbation theory to each gadget individually. A gadget’s simulator Hamiltonian is

\[ H^u = H_0^u + V^u, \]

where \( H_0^u = \Delta Q^u \) penalizes the mediator qubit for being in the state \( |1\rangle \), and \( V^u \) is a perturbation. With the proper choice of \( V^u \) the effective Hamiltonian on the low-energy subspace, in which the mediator qubit \( u \) is in the state \( |0\rangle \), approximates \( H^u \) with an error \( \epsilon \). Furthermore, this effective Hamiltonian can be obtained from \( H^u \) via an approximate Schrieffer-Wolff transformation, that is, \( H_{\text{target}}^u = P^u e^{S^u} (H_0^u + V^u) e^{-S^u} P^u + O(\epsilon J) \) for some anti-hermitian \( S^u \) satisfying \( P^u S^u P^u = Q^u S^u Q^u = 0 \).

Combining the local gadgets together we get as a candidate for the simulator Hamiltonian \( H = H_0 + V + H_{\text{else}} \) with \( H_0 = \sum_u H_0^u \) and \( V = \sum_u V^u \). Let \( \lambda(H) \) and \( \lambda(H_{\text{target}}) \) be the ground-state energy of \( H \) and \( H_{\text{target}} \) respectively. We prove that \( \lambda(H) \) approximates \( \lambda(H_{\text{target}}) \) with a small extensive error by constructing a global unitary transformation \( e^{\lambda} \) mapping \( H \) to \( H_{\text{target}} \) (with a small extensive error), that is, \( H_{\text{target}} = P e^{\lambda} H e^{-\lambda} P + O(\epsilon n J) \) where \( P = \bigotimes_u P^u \) projects onto the subspace in which every mediator qubit is in the state \( |0\rangle \). Given such a transformation one immediately gets an upper bound \( \lambda(H) = \lambda(e^{\lambda} H e^{-\lambda}) \leq \lambda \left( P e^{\lambda} H e^{-\lambda} P \right) = \lambda(H_{\text{target}}) + O(\epsilon n J) \). Here we have taken into account that restricting a Hamiltonian on a subspace can only increase its ground-state energy \([19]\). Making a natural choice \( S = \sum_u S^u \) we prove that \( P e^{\lambda} H e^{-\lambda} P \) contains the desired term \( H_{\text{target}} \) and some cross-gadget terms where \( S^u \) acts on \( H_0^u + V^u \) with \( u \neq v \). Using the ‘independence’ properties of the gadgets and the block-off-diagonality of \( S \) we are able to show that the contribution of these cross-gadget terms are small enough to be absorbed into the error term \( O(\epsilon n) \), see Section II.

In order to prove a matching lower bound, consider the transformed Hamiltonian \( \tilde{H}^u = e^{S^u} H^u e^{-S^u} \), where \( H^u = H_0^u + V^u \). We prove an operator inequality \( \tilde{H}^u \geq I^u \otimes H_{\text{target}}^u + O(\epsilon J) \). Here \( I^u \) is the identity operator acting on the mediator qubit \( u \) and \( O(\epsilon J) \) stands for some operator with norm \( O(\epsilon J) \). Intuitively one should expect this inequality to be true since the \( P \)-block of \( H_{\text{target}}^u \) approximates \( H_{\text{target}}^u \) with an error \( O(\epsilon J) \), the \( Q \)-block of \( H^u \) contains a large energy penalty \( \Delta \), and the off-diagonal blocks \( PH^u Q \) are small by definition of the Schrieffer-Wolff transformation. Using the unitarity of \( e^{\lambda} \) and smallness of \( S^u \) we transform the above inequality into \( H^u \geq \tilde{H}^u \otimes H_{\text{target}}^u + O(\epsilon n J) \) which implies \( H \geq I \otimes H_{\text{target}} + O(\epsilon n J) \) and thus gives \( \lambda(H) \geq \lambda(H_{\text{target}}) + O(\epsilon n J) \). These arguments are filled in at the beginning of Section II.

Our results will be stated for two different mappings \( H_{\text{target}} \rightarrow H \) corresponding to two different gadgets, the one reducing the locality parameter \( k \) by a factor of 2, and the other reducing \( k = 3 \) to \( k = 2 \). By composing these mappings we arrive at Theorem 1.

Before proceeding with the details, let us make a few remarks about generalizations of this technique. We expect that similar results can be obtained for other perturbation gadgets in the literature (see e.g. \([11, 13, 15]\)), since these gadgets are all designed to work independently, i.e. a term in the target Hamiltonian is replaced by some local perturbed Hamiltonian \( H \) and cross-gadgets terms should have small contributions in the perturbation expansion. For Hamiltonians \( H \) of direct interest in many-body physics, we expect that it will also be possible to identify a gadget sub-structure \( H = \sum_u H^u \) such that \( H^u \) gives rise to \( H_{\text{target}} \) and cross-gadget contributions are small. For generic perturbed Hamiltonians, cross-gadget terms may not be small, which implies that the effect of the perturbations must be analyzed globally. We will consider such an analysis in a future paper \([16]\).

Now we state two Lemmas used in the proof. The two Lemmas together can be regarded as an infinitesimal version of the Lieb-Robinson bound that governs time evolution of a local observable under a local Hamiltonian, see e.g. \([17, 18]\).

**Lemma 1.** Let \( S \) be an anti-hermitian operator. Define a superoperator \( L \) such that \( L(X) = [S, X] \) and \( L^0[X] = X \). For any operator \( H \) define \( r_0(H) = \|e^S H e^{-S}\| = \|H\| \), \( r_1(H) = \|e^S H e^{-S} - H\| \), and

\[
r_k(H) = \|e^S H e^{-S} - \sum_{p=0}^{k-1} \frac{1}{p!} L^p(H)\|, \quad k \geq 2,
\]

where \( \|\cdot\| \) is the operator norm. Then for all \( k \geq 0 \) one has

\[
r_k(H) \leq \frac{1}{k!} \|L^k(H)\|.
\]

Using this Lemma one can show that
Lemma 2. Let $S$ and $H$ be any $O(1)$-local operators acting on $n$ qubits with an interaction strengths $J_S$ and $J_H$ respectively. Let each qubit be acted upon non-trivially by $O(1)$ terms of $H$ and $S$. Then for any $k = O(1)$ one has

$$\| L^k(H) \| = O(n \cdot J_S^k J_H^k).$$

(3)

The proofs are rather elementary and can be found in the Appendix.

I. THE GADGETS

We shall use two types of gadgets proposed in [3], namely, the subdivision gadget and the 3-to-2-local gadget. The former will be used to break $k$-local interactions down to 3-local interactions while the latter breaks 3-local interactions up into 2-local interactions. A notational comment: in this section, all Hamiltonian operators, and Schrieffer-Wolff operators $S$, refer to a single gadget $u$, and in the remainder of the paper these operators appear with the label $u$; in this section only, for economy, we omit this label.

Subdivision Gadget. Let the target Hamiltonian be a single $k$-body interaction $H_{\text{target}} = JAB$ where $A, B$ act on non-overlapping subsets of $[k/2]$ or less qubits and $\|A\|, \|B\| \leq 1$. Introduce one mediator qubit $u$, choose a parameter $\Delta \gg J$ and define the simulator Hamiltonian $H = H_0 + V$ with

$$H_0 = \Delta |1⟩⟨1|, \quad V = \sqrt{\Delta J/2} X_u \otimes (-A + B) + V_{\text{extra}}.$$  

(4)

Here $V_{\text{extra}} = (J/2)(A^2 + B^2)$ acts trivially on the mediator qubit. Note that $H$ contains only $([k/2] + 1)$-body interactions. The purpose of the term $V$ is to induce transitions $|0⟩_u → |1⟩_u → |0⟩_u$ in the second order of perturbation theory, see Fig. 1, such that the corresponding effective Hamiltonian is proportional to $(-A + B)^2$ containing the desired term $AB$ and unwanted terms $A^2, B^2$ which we cancel by $V_{\text{extra}}$. Next we define

$$S = -i \sqrt{\frac{J}{2\Delta}} Y_u \otimes (-A + B).$$

(5)

One can check that $S$ is the Schrieffer-Wolff transformation truncated at the first order, i.e. $S = S_1$ where $S_1$ is defined in Eq. (23) in the Appendix. We can calculate $Pe^{S}He^{-S}P$ using the expansion in Lemma 1. A straightforward calculation shows that

$$e^{S}He^{-S} = \left( H + [S, H] + \frac{1}{2}([S, [S, H]]) \right) + O(J^{3/2} \Delta^{-1/2}) = \begin{bmatrix} H_{\text{target}} & 0 \\ 0 & \Delta I + O(J) \end{bmatrix} + O(J^{3/2} \Delta^{-1/2}),$$

(6)

where we used that $[S, V_{\text{extra}}] = 0$. The upper and lower blocks correspond to the subspaces $P$ and $Q = I - P$ respectively. Thus, $Pe^{S}He^{-S}P$ is close to $H_{\text{target}} = JAB$, as desired; the error can be made $O(cJ)$ by choosing $\Delta = Jc^{-2}$.

3-to-2-local Gadget. Let the target Hamiltonian be a single 3-body interaction, $H_{\text{target}} = JABC$, where $A, B, C$ are one-qubit operators acting on different qubits and $\|A\|, \|B\|, \|C\| \leq 1$. Introduce one mediator qubit $u$, choose $\Delta \gg J$ and define the simulator Hamiltonian $H = H_0 + V$ with $H_0 = \Delta |1⟩⟨1|_u$,

$$V = V_d + V_{\text{od}} + V_{\text{extra}}, \quad V_d = -\Delta^2 J^2/2 |1⟩_u ⟨1|_u \otimes C, \quad V_{od} = \frac{\Delta^2 J^2}{\sqrt{2}} X_u \otimes (-A + B),$$

(7)

and $V_{\text{extra}} = \Delta^{1/3}J^{2/3}(-A + B)^2/2 + J(A^2 + B^2)C/2$. Note that $H$ contains only 2-body interactions. The purpose of the term $V$ is to induce transitions $|0⟩_u → |1⟩_u → |1⟩_u → |0⟩_u$ in the third order of perturbation theory, see Fig. 1, such that the corresponding contribution to the effective Hamiltonian is proportional to $(-A + B)^2C$ which coincides with $ABC$ up to some unwanted terms which are canceled by $V_{\text{extra}}$. We define

$$S = -ix \sqrt{\frac{J}{\Delta}} Y_u \otimes (-A + B) \left[ I + xC + x^2C^2 - \frac{2x^2}{3} (-A + B)^2 \right], \quad x = \left( \frac{J}{\Delta} \right)^{1/2}.$$  

(8)

One can check that $S$ is the Schrieffer-Wolff transformation truncated at the third order, i.e., $S = S_1 + S_2 + S_3$, see Eq. (23) in the Appendix. We calculate the effective Hamiltonian $Pe^{S}He^{-S}P$. Let us first estimate an error resulting from cutting off the expansion, see Lemma 1. Recalling that $L = [S, \cdot]$ one gets

$$\| Pe^{S}He^{-S}P - P \left( H + [S, H] + \frac{1}{2}[[S, [S, H]]] \right) P \| \leq \frac{1}{6} \| PL^3(H) P \| + \frac{1}{24} \| L^4(H) \|.$$  

(9)
We note that $PL^3(H)P = PL^3(V_{\text{act}})P$ since each application of $S$ flips the mediator qubit and a non-zero contribution comes only from the terms with an even number of flips. Using a bound $\|S\| = O(\epsilon)$, see Eq. (5), one can upper-bound the r.h.s. in Eq. (9) as $O(J^{4/3}\Delta^{-1/3})$. A direct but lengthy calculation shows that

$$e^SHe^{-S} = \left(H + [S,H] + \frac{1}{2}[S,[S,H]] + \frac{1}{6}[S,[S,[S,H]]]\right) + O(J^{4/3}\Delta^{-1/3})$$

$$= \left[\lambda_{\text{target}} H_{\text{target}} + \frac{1}{\Delta} I + O(\Delta J^{3/4} J^{-1/3})\right] + O(J^{4/3}\Delta^{-1/3}), \tag{10}$$

where $H_{\text{target}} = JABC$, as desired. The error $O(J^{4/3}\Delta^{-1/3})$ in $H_{\text{target}}$ can be made $O(\epsilon J)$ by choosing $\Delta = J\epsilon^{-3}$.

II. COMBINING THE GADGETS TOGETHER

Let $H_{\text{target}} = \sum_u H_{\text{target}}^u + H_{\text{else}}$, where each term $H_{\text{target}}^u$ can be dealt with using one of the gadgets described above. The simulator Hamiltonian is $H = \sum_u H^u + H_{\text{else}}$ where $H^u$ is the simulator constructed for a gadget $u$ as above. Using Eqs. (6,10) one gets the inequality $e^SHe^{-S} \geq \sum_u H_{\text{target}}^u + O(\epsilon J)$ which yields $H^u \geq e^{-S} (I^u \otimes H_{\text{target}}^u) e^S + O(\epsilon J)$. Applying Lemma 1 one gets $\|e^{-S} (I^u \otimes H_{\text{target}}^u) e^S - I^u \otimes H_{\text{target}}^u\| \leq \|S\|_u I^u \otimes H_{\text{target}}^u\| = O(\epsilon J)$, see Eqs. (3,8). It follows that $H^u \geq I^u \otimes H_{\text{target}} + O(\epsilon J)$. Summing up these inequalities over all gadgets one arrives at $H \geq I \otimes H_{\text{target}} + O(\epsilon\Delta)\|$, where $I$ acts on the mediator qubits. Thus

$$\lambda(H) \geq \lambda(H_{\text{target}}) + O(\epsilon\Delta). \tag{11}$$

Bounding Cross-Gadget Contributions. Let $P = \bigotimes_u P^u$ be the projector on the subspace in which every mediator qubit is in the state $|0\rangle$. Define $S = \sum_u S^u$ where $S^u$ is constructed using Eqs. (5,8). Below we shall prove that

$$\|Pe^SHe^{-S}P - H_{\text{target}}\| = O(\epsilon\Delta). \tag{12}$$

Then one can get an upper bound on $\lambda(H)$ by observing that

$$\lambda(H) = \lambda(e^SHe^{-S}) \leq \lambda(Pe^SHe^{-S}P) = \lambda(H_{\text{target}}) + O(\epsilon\Delta). \tag{13}$$

Combining Eqs. (11,13) one gets $|\lambda(H) - \lambda(H_{\text{target}})| = O(\epsilon\Delta)$ which is the desired result. It remains to prove Eq. (12). The idea is to bound the cross-gadget terms using Lemma 1 and Lemma 2. Two important properties (valid for both gadgets) will be used repeatedly in this argument: (1) $S^u$ always flips a mediator qubit $u$; (2) For $u \neq v$ one has $[P^u,H^v] = 0$, $[P^u,S^v] = 0$, $[H^u_0,S^v] = 0$. This latter property essentially captures the independent action of the local gadgets.

Let us start with the subdivision gadget. Recall that we have chosen $\Delta = J\epsilon^{-2}$. From Eq. (3) we can see that $S$ is a $O(1)$-local operator with an interaction strength $O(\epsilon)$. Applying Lemma 1 we get

$$\|Pe^SHe^{-S}P - H_{\text{target}}\| \leq \|S,H_{\text{else}}\| + \sum_u \|P(H^u + [S,H^u] + \frac{1}{2}[S,[S,H^u]])P - H_{\text{target}}^u\| + \frac{1}{6}\|L^3(H)\|, \tag{14}$$

Lemma 2 gives $||[S,H_{\text{else}}]\| = O(\epsilon\Delta)$ and $||L^3(H)\| = O(\epsilon^3\Delta\|) = O(\epsilon\Delta)$. Properties (1),(2) above imply $P[S^u,H^v] = 0$ for $u \neq v$ and that $P[S^{u_1},[S^{u_2},H^v]] = 0$ unless $u_1 = u_2$. Property (2) implies that $P[S^u,[S^v,H^w]] = 0$ for $u \neq v$ and thus the only non-zero cross-talk term could be $P[S^v,[S^v,V^u]]P$ where $u \neq v$. Using the explicit form of $V^u$, see Eq. (1), and property (1) one concludes that $P[S^v,[S^v,V^u]]P = P[S^v,[S^v,V_{\text{extra}}^u]]P$. 
By construction of the individual gadgets, the contribution of the “diagonal” terms (those in which $H^u$ and $S^u$ belong to the same gadget) is $O(enJ)$, see Eq. (3). Combining these observations together we arrive at

$$\|Pe^SHe^{-S}P - H_{\text{target}}\| \leq O(enJ) + \sum_{u \neq v} \| P[S^u, S^u, V^u]\| P\|$$

(15)

Now, note that for any $u$ there exist only $O(1)$ mediator qubits $v$ such that $[S^v, V^u] \neq 0$. Since $V^u_{\text{extra}}$ has norm $O(J)$ the contribution of the cross-talk terms is $O(n^2eJ)$ and we arrive at Eq. (12).

Let us do a similar analysis for the 3-to-2-local gadget. Recall that we have chosen $\Delta = J\epsilon^{-3}$. From Eq. (5) we see that $S$ is a $O(1)$-local operator with interaction strength $O(\epsilon)$. Applying Lemma 1 we get

$$\| Pe^SHe^{-S}P - H_{\text{target}}\| \leq \| [S, H_{\text{else}}] \| + \sum_{u} \| P (H^u + [S, H^u] + \frac{1}{2} [S, [S, H^u]]) P - H^u_{\text{target}} \|$$

$$+ \frac{1}{3!} \| PL^3(H)P\| + \frac{1}{4!} \| L^4(H)\|.$$  

(16)

Lemma 2 gives $\| [S, H_{\text{else}}] \| = O(enJ)$, $\| L^4(H)\| = O(\epsilon^4\Delta n) = O(enJ)$. Property (1) implies $PL^3(H_0)P = 0$. Taking into account that $V$ has interaction strength $\Delta^{1/3}J^{1/3} = \Delta_*$, see Eq. (7), and applying Lemma 2 we get $\| PL^3(H)P\| = \| PL^3(V)P\| = O(n^2\Delta_*) = O(enJ)$. Repeating the same arguments as for the subdivision gadget we conclude that the only cross-talk terms contributing to Eq. (16) are $P [S^v, [S^v, V^u]] P$ where $u \neq v$. Using the explicit form of $V^u$, see Eq. (1), one concludes that $P [S^v, S^v, V^u] P = P [S^v, S^v, V^u_{\text{extra}}] P$ so we again arrive at the bound Eq. (15). By definition, $V^u_{\text{extra}}$ has norm $O(\Delta^{1/3}J^{2/3}) = O(J\epsilon^{-1})$ and $S^v$ has norm $O(\epsilon)$. Making use of the properties of $H_{\text{target}}$ we conclude that the contribution of the cross-talk terms is $O(n\epsilon J)$ and we arrive at Eq. (12).

III. SIMULATION OVERHEAD

Let us estimate the overall increase of the interaction strength associated with $m$ levels of simulation using the subdivision gadget. Let $H_i$ be a Hamiltonian at a level $i$ of the simulation such that $H_0 = H_{\text{target}}$ and $H_m$ is 3-local. Accordingly, $H_{\text{target}}$ can be $k$-local where $k \sim 2^m$. The overall number of mediator qubits one needs for the simulation is $O(n2^{O(k)})$. For simplicity one can add all these qubits to the system from the beginning by letting $H_{\text{target}}$ to act trivially on them. It allows us to assume that at every level of simulation we have $n' = O(n2^{O(k)})$ qubits. Let $\lambda_i$ be the ground state energy of $H_i$. Let $J_i$ be the interaction strength of $H_i$. In order to make $|\lambda_{i+1} - \lambda_i| \sim n' \delta$ it suffices to choose $J_{i+1} = \delta^{-2}J_i^3$. Accordingly, $\delta^{-1}J_m = (\delta^{-1}J_0)^{3^m}$ and thus $J_m = O(\log k) \sim J_0^{poly(k)} \delta^{-poly(k)}$. Choosing $\delta = 2^{-O(k)}\epsilon$ one can make the overall error $|\lambda_0 - \lambda_m| \sim \epsilon n$. Assuming that $J_0 = O(1)$ we get $J_{\text{final}} \sim (2\epsilon^{-1})^{poly(k)}$.

It may be possible to improve this exponential scaling by using a direct $k$-to-$2$-local gadget.

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APPENDIX

Proof of Lemma 1. For any real $t \geq 0$, let $H(t) = e^{St}He^{-St}$. Define an auxiliary quantity

$$r_k(H, t) = \| H(t) - \sum_{p=0}^{k-1} \frac{1}{p!} L^p(H) \|.$$  

(17)

Let us get an upper bound on the increment $r_k(H, t + \delta t) - r_k(H, t)$. First of all notice that

$$H(t + \delta t) - H(t) = \delta t e^{St}L(H)e^{-St} + O((\delta t)^2).$$  

(18)
Secondly, for any \( k \geq 1 \) one has
\[
\sum_{p=0}^{k-1} \frac{(t + \delta t)^p}{p!} L^p(H) - \sum_{p=0}^{k-1} \frac{t^p}{p!} L^p(H) = \frac{\delta t}{k} \sum_{p=0}^{k-2} \frac{t^p}{p!} L^p(L(H)) + O((\delta t)^2). \tag{19}
\]
(if \( k = 1 \) then there are no \( O(\delta t) \) terms on the right hand side). Applying the triangle inequality one gets
\[
\delta t (H, t + \delta t) - \delta t (H, t) \leq \delta t (L(H), t) + O((\delta t)^2). \tag{20}
\]
Since \( r_k(H, t) \) is a continuous function of \( t \), it is legitimate to add up the inequalities Eq. (20) for \( t = 0, \delta t, 2\delta t, \ldots, s \), take a limit \( \delta t \to 0 \), and replace the resulting sum by an integral, which yields
\[
r_k(H, t) \leq \int_0^s dt r_{k-1}(L(H), t) \quad \text{if } k \geq 1, \quad \text{and} \quad r_0(H, s) = \|H\|. \tag{21}
\]
Applying this upper bound recursively and evaluating the integrals one arrives at
\[
r_k(H, t) \leq \|L^k(H)\| \cdot \frac{t^k}{(k)!} \quad \text{for all } k \geq 0. \tag{22}
\]
Since \( r_k(H) = r_k(H, 1) \) Eq. (22) proves the lemma.

**Proof of Lemma 3.** Represent \( S \) and \( H \) as a sum of local operators \( S = \sum_{i=1}^{K'} S_i \) and \( H = \sum_{j=1}^K H_j \) such that any \( S_i, H_j \) act on \( O(1) \) qubits and any qubit is acted on by \( O(1) \) operators \( S_i, H_j \). Let us use the term \textit{elementary commutator of order} \( k \) for a multiple commutator that involves some \( H_j \) and \( k \) operators \( S_i \). For example, \([S_1, [S_2, H_1]]\) is an elementary commutator of order \( 2 \). Note that a commutator of any \( O(1) \)-local operators is again a \( O(1) \)-local operator. Therefore for any constant \( k \) the number of non-zero elementary commutators of order \( k \) contributing to \( L^k(H) \) can be bounded as \( O(n) \). Each elementary commutator of order \( k \) has a norm at most \( 2^k J_k S J_H \). Applying the triangle inequality to \( \|L^k(H)\| \) we get Eq. (3).

**SYSTEMATIC SOLUTION FOR THE SCHRIEFFER-WOLFF TRANSFORMATION**

One can note that the equation \( P e^{s(H_0 + \beta V)} e^{-s} Q = 0 \) has a unique solution in terms of a formal Taylor series \( S = \sum_{p=1}^\infty S_p \beta^p \); the series coefficients \( S_p \) can be straightforwardly computed. In the gadgets we have used an approximate version of \( S \) obtained by truncating the Taylor series at the first (subdivision gadget) or the third order (3-to-2-local gadget). Introducing operators \( V_d = P V P + Q V Q, \ V_{od} = P V Q + Q V P \) and linear maps \( L_0 = [H_0, \cdot], L_p = [S_p, \cdot] \) one can derive that
\[
S_1 = L_0^{-1}(V_{od}), \quad S_2 = L_0^{-1} L_1(V_{d}), \quad S_3 = -\frac{1}{3} L_0^{-1} L_1^3(H_0) + L_0^{-1} L_2(V_{d}). \tag{23}
\]

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[19] By abuse of notation, \( P e^S H e^{-S} P \) denotes the restriction of the operator \( e^S H e^{-S} \) onto the subspace \( P \).