Perturbative gadgets at arbitrary orders

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Adiabatic quantum algorithms are often most easily formulated using many-body interactions. However, experimentally available interactions are generally two-body. In 2004, Kempe, Kitaev, and Regev introduced perturbative gadgets, by which arbitrary three-body effective interactions can be obtained using Hamiltonians consisting only of two-body interactions. These three-body effective interactions arise from the third order in perturbation theory. Since their introduction, perturbative gadgets have become a standard tool in the theory of quantum computation. Here we construct generalized gadgets so that one can directly obtain arbitrary k-body effective interactions from two-body Hamiltonians. These effective interactions arise from the kth order in perturbation theory.

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I. PERTURBATIVE GADGETS

Perturbative gadgets were introduced to construct a two-local Hamiltonian whose low-energy effective Hamiltonian corresponds to a desired three-local Hamiltonian. They were originally developed by Kempe, Kitaev, and Regev in 2004 to prove the QMA-completeness[1] of the two-local Hamiltonian problem and to simulate three-local adiabatic quantum computation using two-local adiabatic quantum computation [1]. Perturbative gadgets have subsequently been used to simulate spatially nonlocal Hamiltonians using spatially local Hamiltonians [2], and to find a minimal set of interactions for universal adiabatic quantum computation [3]. It was also pointed out in [6] that perturbative gadgets can be used recursively to obtain k-local effective interactions using a 2–local Hamiltonian. Here we generalize perturbative gadgets to directly obtain arbitrary k-local effective interactions by a single application of kth order perturbation theory. Our formulation is based on a perturbation expansion due to Bloch [4].

A k-local operator is one consisting of interactions between at most k qubits. A general k-local Hamiltonian on n qubits can always be expressed as a sum of r terms,

$$H^{\mathrm{comp}} = \sum_{s=1}^{r} c_s H_s \tag{1}$$

with coefficients c_s, where each term H_s is a k-fold tensor product of Pauli operators. That is, H_s couples some set of k qubits according to

$$H_s = \sigma_{s,1}\sigma_{s,2}\cdots\sigma_{s,k}, \tag{2}$$

where each operator $\sigma_{s,j}$ is of the form

$$\sigma_{s,j} = \hat{n}_{s,j}\cdot\vec{\sigma}_{s,j}, \tag{3}$$

where $\hat{n}_{s,j}$ is a unit vector in $\mathbb{R}^3$, and $\vec{\sigma}_{s,j}$ is the vector of Pauli matrices operating on the jth qubit in the set of k qubits acted upon by H_s.

We wish to simulate H^{comp} using only two-local interactions. To this end, for each term H_s, we introduce k ancilla qubits, generalizing the technique of [1]. There are then rk ancilla qubits and n computational qubits, and we choose the gadget Hamiltonian as

$$H^{\mathrm{gad}} = \sum_{s=1}^{r} H_s^{\mathrm{anc}} + \lambda\sum_{s=1}^{r} V_s, \tag{4}$$

where

$$H_s^{\mathrm{anc}} = \sum_{1\le i<j\le k} \frac{1}{2}(I - Z_{s,i}Z_{s,j}), \tag{5}$$

and

$$V_s = \sum_{j=1}^{k} c_{s,j}\sigma_{s,j}\otimes X_{s,j}. \tag{6}$$

and

$$c_{s,j} = \begin{cases} c_s & \text{if } j=1 \\ 1 & \text{otherwise.} \end{cases}$$

For each s there is a corresponding register of k ancilla qubits. The operators $X_{s,j}$ and $Z_{s,j}$ are Pauli X and Z operators acting on the jth ancilla qubit in the ancilla register associated with s. For each ancilla register, the ground space of H_s^{anc} is the span of $|000\cdots\rangle$ and $|111\cdots\rangle$ (see Fig. 1). λ is the small parameter in which the perturbative analysis is carried out.

For each s, the operator

$$X_s^{\otimes k} = X_{s,1}\otimes X_{s,2}\otimes\cdots\otimes X_{s,k} \tag{7}$$

acting on the k ancilla qubits in the register s commutes with H^{gad}. Since there are r ancilla registers, H^{gad} can be block diagonalized into 2^r blocks, where each register is in either the $+1$ or -1 eigenspace of its $X_s^{\otimes k}$. In this paper, we analyze

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[1]For a definition of QMA (Quantum Merlin-Arthur) and QMA-completeness see [7].

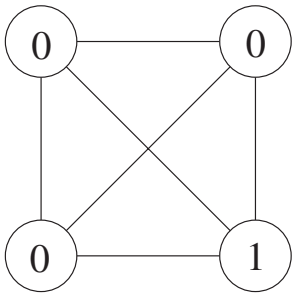

FIG. 1. The ancilla qubits are all coupled together using ZZ couplings. This gives a unit energy penalty for each pair of unaligned qubits. If there are k bits, of which j are in the state $|1\rangle$ and the remaining $k-j$ are in the state $|0\rangle$, then the energy penalty is $j(k-j)$. In the example shown in this diagram, the 1 and 0 labels indicate that the qubits are in the state $|0001\rangle$, which has energy penalty 3.

only the block corresponding to the +1 eigenspace for every register. This +1 block of the gadget Hamiltonian is a Hermitian operator, that we label H_+^{gad}. We show that the effective Hamiltonian on the low-energy eigenstates of H_+^{gad} approximates H^{comp}. For many purposes this is sufficient. For example, suppose one wishes to simulate a k-local adiabatic quantum computer using a two-local adiabatic quantum computer. If the initial state of the computer lies within the all +1 subspace, then the system will remain in this subspace throughout its evolution. To put the initial state of the system into the all +1 subspace, one can initialize each ancilla register to the state

$$|+\rangle = \frac{1}{\sqrt{2}}(|000\ldots\rangle + |111\ldots\rangle), \tag{8}$$

which is the ground state of $\Sigma_s H_s^{\mathrm{anc}}$ within the +1 subspace. Given the extensive experimental literature on the preparation of states of the form $|+\rangle$, sometimes called cat states, a supply of such states seems a reasonable resource to assume.

The purpose of the perturbative gadgets is to obtain k-local effective interactions in the low-energy subspace. To quantify this, we use the concept of an effective Hamiltonian. We define this to be

$$H_{\mathrm{eff}}(H,d) \equiv \sum_{j=1}^{d} E_j |\psi_j\rangle\langle\psi_j|, \tag{9}$$

where $|\psi_1\rangle,\ldots,|\psi_d\rangle$ are the d lowest energy eigenstates of a Hamiltonian H, and $E_1,\ldots,E_d$ are their energies.

In Sec. III, we calculate $H_{\mathrm{eff}}(H_+^{\mathrm{gad}},2^n)$ perturbatively to kth order in λ. To do this, we write H^{gad} as

$$H^{\mathrm{gad}} = H^{\mathrm{anc}} + \lambda V, \tag{10}$$

where

$$H^{\mathrm{anc}} = \sum_{s=1}^{r} H_s^{\mathrm{anc}} \tag{11}$$

and

$$V = \sum_{s=1}^{r} V_s. \tag{12}$$

We consider H^{anc} to be the unperturbed Hamiltonian and λV to be the perturbation. We find that λV perturbs the ground space of H^{anc} in two separate ways. The first is to shift the energy of the entire space. The second is to split the degeneracy of the ground space. This splitting arises at kth order in perturbation theory, because the lowest power of λV that has nonzero matrix elements within the ground space of H^{anc} is the kth power. It is this splitting which allows the low-energy subspace of H_+^{gad} to mimic the spectrum of H^{comp}.

It is convenient to analyze the shift and the splitting separately. To do this, we define

$$\tilde{H}_{\mathrm{eff}}(H,d,\Delta) \equiv H_{\mathrm{eff}}(H,d) - \Delta\Pi, \tag{13}$$

where Π is the projector onto the support of $H_{\mathrm{eff}}(H,d)$. Thus, $\tilde{H}_{\mathrm{eff}}(H,d,\Delta)$ differs from $H_{\mathrm{eff}}(H,d)$ only by an energy shift of magnitude Δ. The eigenstates of $\tilde{H}_{\mathrm{eff}}(H,d,\Delta)$ are identical to the eigenstates of $H_{\mathrm{eff}}(H,d)$, as are all the gaps between eigenenergies. The rest of this paper is devoted to showing that, for any k-local Hamiltonian H^{comp} acting on n qubits, there exists some function $f(\lambda)$ such that

$$\tilde{H}_{\mathrm{eff}}(H_+^{\mathrm{gad}},2^n,f(\lambda)) = \frac{-k(-\lambda)^k}{(k-1)!} H^{\mathrm{comp}} \otimes P_+ + O(\lambda^{k+1}) \tag{14}$$

for sufficiently small λ. Here P_+ is an operator acting on the ancilla registers, projecting each one into the state $|+\rangle$. To obtain Eq. (14) we use a formulation of degenerate perturbation theory due to Bloch [4,5], which we describe in the next section.

II. PERTURBATION THEORY

Suppose we have a Hamiltonian of the form

$$H = H^{(0)} + \lambda V, \tag{15}$$

where $H^{(0)}$ has a d-dimensional degenerate ground space $\mathcal{E}^{(0)}$ of energy zero. As discussed in [5,6], the effective Hamiltonian for the d lowest eigenstates of H can be obtained directly as a perturbation series in V. However, for our purposes it is more convenient to use an indirect method due to Bloch [4,5], which we now describe. As shown in Appendix B, the perturbative expansions converge provided that

$$\|\lambda V\| < \frac{\gamma}{4}, \tag{16}$$

where γ is the energy gap between the eigenspace in question and the next-nearest eigenspace, and $\|\cdots\|$ denotes the operator norm.[2]

Let $|\psi_1\rangle,\ldots,|\psi_d\rangle$ be the d lowest energy eigenstates of H, and let $E_1,\ldots,E_d$ be their energies. For small perturbations, these states lie primarily within $\mathcal{E}^{(0)}$. Let

[2]For any linear operator M, $\|M\| \equiv \max_{|\langle\psi|\psi\rangle|=1} |\langle\psi|M|\psi\rangle|$.

$$|\alpha_j\rangle = P_0|\psi_j\rangle, \tag{17}$$

where P_0 is the projector onto $\mathcal{E}^{(0)}$. For λ satisfying (16), the vectors $|\alpha_1\rangle,\ldots,|\alpha_d\rangle$ are linearly independent, and there exists a linear operator $\mathcal{U}$ such that

$$|\psi_j\rangle = \mathcal{U}|\alpha_j\rangle \quad \text{for } j=1,2,\ldots,d \tag{18}$$

and

$$\mathcal{U}|\phi\rangle = 0 \quad \text{for} \quad |\phi\rangle \in \mathcal{E}^{(0)\perp}. \tag{19}$$

Note that $\mathcal{U}$ is in general nonunitary. Let

$$\mathcal{A} = \lambda P_0 V \mathcal{U}. \tag{20}$$

As shown in [4,5] and recounted in Appendix A, the eigenvectors of $\mathcal{A}$ are $|\alpha_1\rangle,\ldots,|\alpha_d\rangle$, and the corresponding eigenvalues are $E_1,\ldots,E_d$. Thus,

$$H_{\text{eff}} = \mathcal{U}\mathcal{A}\mathcal{U}^\dagger. \tag{21}$$

$\mathcal{A}$ and $\mathcal{U}$ have the following perturbative expansions. Let S^l be the operator

$$S^l = \begin{cases} \sum_{j\neq 0} \dfrac{P_j}{(-E_j^{(0)})^l} & \text{if } l>0, \\ -P_0 & \text{if } l=0, \end{cases} \tag{22}$$

where P_j is the projector onto the eigenspace of $H^{(0)}$ with energy $E_j^{(0)}$. (Recall that $E_0^{(0)}=0$.) Then

$$\mathcal{A} = \sum_{m=1}^{\infty} \mathcal{A}^{(m)}, \tag{23}$$

where

$$\mathcal{A}^{(m)} = \lambda^m \sum_{(m-1)} P_0 V S^{l_1} V S^{l_2} \cdots V S^{l_{m-1}} V P_0, \tag{24}$$

and the sum is over all non-negative integers $l_1\cdots l_{m-1}$ satisfying

$$l_1 + \cdots + l_{m-1} = m-1, \tag{25}$$

$$l_1 + \cdots + l_p \geq p \quad (p=1,2,\ldots,m-2). \tag{26}$$

Similarly, $\mathcal{U}$ has the expansion

$$\mathcal{U} = P_0 + \sum_{m=1}^{\infty} \mathcal{U}^{(m)}, \tag{27}$$

where

$$\mathcal{U}^{(m)} = \lambda^m \sum_{(m)} S^{l_1} V S^{l_2} V \cdots V S^{l_m} V P_0, \tag{28}$$

and the sum is over

$$l_1 + \cdots + l_m = m, \tag{29}$$

$$l_1 + \cdots + l_p \geq p \quad (p=1,2,\ldots,m-1). \tag{30}$$

In Appendix A we derive the expansions for $\mathcal{U}$ and $\mathcal{A}$, and in Appendix B we prove that condition (16) suffices to ensure convergence. The advantage of the method of [4] over the direct approach of [6] is that $\mathcal{A}$ is an operator whose support is strictly within $\mathcal{E}^{(0)}$, which makes some of the calculations more convenient.

III. ANALYSIS OF GADGET HAMILTONIAN

Before analyzing H^{gad} for a general k-local Hamiltonian, we first consider the case where H^{comp} has one coefficient $c_s=1$ and all the rest equal to 0. That is,

$$H^{\text{comp}} = \sigma_1\sigma_2\cdots\sigma_k, \tag{31}$$

where for each j, $\sigma_j = \hat{n}_j\cdot\vec{\sigma}_j$ for some unit vector $\hat{n}_j$ in $\mathbb{R}^3$. The corresponding gadget Hamiltonian is thus

$$H^{\text{gad}} = H^{\text{anc}} + \lambda V, \tag{32}$$

where

$$H^{\text{anc}} = \sum_{1\leq i<j\leq k} \frac{1}{2}(I - Z_iZ_j) \tag{33}$$

and

$$V = \sum_{j=1}^{k} \sigma_j \otimes X_j. \tag{34}$$

Here σ_j acts on the jth computational qubit, and X_j and Z_j are the Pauli X and Z operators acting on the jth ancilla qubit. We use kth-order perturbation theory to show that $\tilde{H}^{\text{eff}}(H_+^{\text{gad}},2^k,\Delta)$ approximates H^{comp} for appropriate Δ.

We start by calculating $\mathcal{A}$ for H_+^{gad}. For H^{anc}, the energy gap is $\gamma=k-1$, and $\|V\|=k$, so by condition (16), we can use perturbation theory provided λ satisfies

$$\lambda < \frac{k-1}{4k}. \tag{35}$$

Because all terms in $\mathcal{A}$ are sandwiched by P_0 operators, the nonzero terms in $\mathcal{A}$ are ones in which the m powers of V take a state in $\mathcal{E}^{(0)}$ and return it to $\mathcal{E}^{(0)}$. Because we are working in the +1 eigenspace of $X^{\otimes k}$, an examination of Eq. (33) shows that $\mathcal{E}^{(0)}$ is the span of the states in which the ancilla qubits are in the state $|+\rangle$. Thus, $P_0=I\otimes P_+$, where P_+ acts only on the ancilla qubits, projecting them onto the state $|+\rangle$. Each term in V flips one ancilla qubit. To return to $\mathcal{E}^{(0)}$, the powers of V must either flip some ancilla qubits and then flip them back, or they must flip all of them. The latter process occurs at kth order and gives rise to a term that mimics H^{comp}. The former process occurs at many orders, but at orders k and lower gives rise only to terms proportional to P_0.

As an example, let us examine $\mathcal{A}$ up to second order for $k>2$,

$$\mathcal{A}^{(\leq 2)} = \lambda P_0 V P_0 + \lambda^2 P_0 V S^1 V P_0. \tag{36}$$

The term P_0VP_0 is zero, because V kicks the state out of $\mathcal{E}^{(0)}$. By Eq. (34) we see that applying V to a state in the ground space yields a state in the energy $k-1$ eigenspace. Substituting this denominator into S^1 yields

$$\mathcal{A}^{(2)} = -\frac{\lambda^2}{k-1} P_0 V^2 P_0. \tag{37}$$

Because V is a sum, V^2 consists of the squares of individual terms of V and cross terms. The cross terms flip two ancilla qubits, and thus do not return the state to the ground space. The squares of individual terms are proportional to the identity, thus

$$\mathcal{A}^{(2)} = \lambda^2 \alpha_2 P_0 \tag{38}$$

for some λ-independent constant α_2. Similarly, at any order $m<k$, the only terms in V^m which project back to $\mathcal{E}^{(0)}$ are those arising from squares of individual terms, which are proportional to the identity. Thus, up to order $k-1$,

$$\mathcal{A}^{(\leq k-1)} = \left(\sum_m \alpha_m \lambda^m \right) P_0, \tag{39}$$

where the sum is over even m between zero and $k-1$ and $\alpha_0, \alpha_2, \ldots$ are the corresponding coefficients.

At kth order there arises another type of term. In V^k there are k-fold cross terms in which each of the terms in V appears once. For example, there is the term

$$\lambda^k P_0 (\sigma_1 \otimes X_1) S^1 (\sigma_2 \otimes X_2) S^1 \cdots S^1 (\sigma_k \otimes X_k) P_0. \tag{40}$$

The product of the energy denominators occurring in the S^1 operators is

$$\prod_{j=1}^{k-1} \frac{1}{-j(k-j)} = \frac{(-1)^{k-1}}{[(k-1)!]^2}. \tag{41}$$

Thus, this term is

$$\frac{(-1)^{k-1}\lambda^k}{[(k-1)!]^2} P_0 (\sigma_1 \otimes X_1)(\sigma_2 \otimes X_2) \cdots (\sigma_k \otimes X_k) P_0, \tag{42}$$

which can be rewritten as

$$\frac{-(-\lambda)^k}{[(k-1)!]^2} P_0 (\sigma_1 \sigma_2 \cdots \sigma_k \otimes X^{\otimes k}) P_0. \tag{43}$$

This term mimics H^{comp}. The fact that all of the S operators in this term are S^1 is a general feature. Any term in $\mathcal{A}^{(k)}$ where $l_1 \cdots l_{k-1}$ are not all equal to 1 either vanishes or is proportional to P_0. This is because such terms contain P_0 operators separated by fewer than k powers of V, and thus the same arguments used for $m<k$ apply.

There are a total of $k!$ terms of the type shown in expression (40). Thus, up to kth order

$$\mathcal{A}^{(\leq k)} = f(\lambda) P_0 + \frac{-k(-\lambda)^k}{(k-1)!} P_0 (\sigma_1 \sigma_2 \cdots \sigma_k \otimes X^{\otimes k}) P_0, \tag{44}$$

which can be written as

$$\mathcal{A}^{(\leq k)} = f(\lambda) P_0 + \frac{-k(-\lambda)^k}{(k-1)!} P_0 (H^{\text{comp}} \otimes X^{\otimes k}) P_0, \tag{45}$$

where $f(\lambda)$ is some polynomial in λ. Note that, up to kth order, $\mathcal{A}$ happens to be Hermitian. The effective Hamiltonian is $\mathcal{U}\mathcal{A}\mathcal{U}^\dagger$, thus by Eq. (45),

$$\begin{aligned} H_{\text{eff}}(H_+^{\text{gad}}, 2^k) &= \mathcal{U} f(\lambda) P_0 \mathcal{U}^\dagger + \mathcal{U} \left(\frac{-k(-\lambda)^k}{(k-1)!} P_0 (H^{\text{comp}} \otimes X^{\otimes k}) P_0 \right. \\ &\quad \left. + O(\lambda^{k+1}) \right) \mathcal{U}^\dagger \\ &= f(\lambda) \Pi + \mathcal{U} \left(\frac{-k(-\lambda)^k}{(k-1)!} P_0 (H^{\text{comp}} \otimes X^{\otimes k}) P_0 \right. \\ &\quad \left. + O(\lambda^{k+1}) \right) \mathcal{U}^\dagger \end{aligned} \tag{46}$$

since $\mathcal{U} P_0 \mathcal{U}^\dagger = \Pi$. Thus,

$$\begin{aligned} \tilde{H}_{\text{eff}}(H_+^{\text{gad}}, 2^k, f(\lambda)) &= \mathcal{U} \left(\frac{-k(-\lambda)^k}{(k-1)!} P_0 (H^{\text{comp}} \otimes X^{\otimes k}) P_0 \right. \\ &\quad \left. + O(\lambda^{k+1}) \right) \mathcal{U}^\dagger. \end{aligned} \tag{47}$$

To order λ^k, we can approximate $\mathcal{U}$ as P_0 since the higher-order corrections to $\mathcal{U}$ give rise to terms of order λ^{k+1} and higher in the expression for $\tilde{H}_{\text{eff}}(H_+^{\text{gad}}, 2^k, f(\lambda))$. Thus,

$$\tilde{H}_{\text{eff}}(H_+^{\text{gad}}, 2^k, f(\lambda)) = \frac{-k(-\lambda)^k}{(k-1)!} P_0 (H^{\text{comp}} \otimes X^{\otimes k}) P_0 + O(\lambda^{k+1}). \tag{48}$$

Using $P_0 = I \otimes P_+$ we rewrite this as

$$\tilde{H}_{\text{eff}}(H_+^{\text{gad}}, 2^k, f(\lambda)) = \frac{-k(-\lambda)^k}{(k-1)!} H^{\text{comp}} \otimes P_+ + O(\lambda^{k+1}). \tag{49}$$

Now let us return to the general case where H^{comp} is a linear combination of k-local terms with arbitrary coefficients c_s, as described in Eq. (1). Now that we have gadgets to obtain k-local effective interactions, it is tempting to eliminate one k-local interaction at a time, by introducing corresponding gadgets one by one. However, this approach does not lend itself to simple analysis by degenerate perturbation theory. This is because the different k-local terms in general act on overlapping sets of qubits. Hence, we instead consider

$$V^{\text{gad}} = \sum_{s=1}^{r} V_s \tag{50}$$

as a single perturbation, and work out the effective Hamiltonian in powers of this operator. The unperturbed part of the total gadget Hamiltonian is thus

$$H^{\text{anc}} = \sum_{s=1}^{r} H_s^{\text{anc}}, \tag{51}$$

which has energy gap $\gamma = k-1$. The full Hamiltonian is

$$H^{\text{gad}} = H^{\text{anc}} + \lambda V^{\text{gad}}, \tag{52}$$

so the perturbation series is guaranteed to converge under the condition

$$\lambda < \frac{k-1}{4\|V^{\mathrm{gad}}\|}. \tag{53}$$

As mentioned previously, we will work only within the simultaneous +1 eigenspace of the $X^{\otimes k}$ operators acting on each of the ancilla registers. In this subspace, H^{anc} has degeneracy 2^n which gets split by the perturbation λV so that it mimics the spectrum of H^{comp}.

Each V_s term couples to a different ancilla register. Hence, any cross term between different V_s terms flips some ancilla qubits in one register and some ancilla qubits in another. Thus, at kth order, nonidentity cross terms between different s cannot flip all k ancilla qubits in any given ancilla register, and they are thus projected away by the P_0 operators appearing in the formula for $\mathcal{A}$. Hence, the perturbative analysis proceeds just as it did when there was only a single nonzero c_s, and one finds,

$$\tilde{H}_{\mathrm{eff}}(H_+^{\mathrm{gad}},2^n,f(\lambda)) = \frac{-k(-\lambda)^k}{(k-1)!}P_0\left(\sum_{s=1}^{r} c_s H_s \otimes X_s^{\otimes k}\right)P_0 + O(\lambda^{k+1}), \tag{54}$$

where $X_s^{\otimes k}$ is the operator $X^{\otimes k}$ acting on the register of k ancilla qubits corresponding to a given s, and $f(\lambda)$ is some polynomial in λ of degree at most k. Note that coefficients in the polynomial $f(\lambda)$ depend on H^{comp}. As before, this can be rewritten as

$$\tilde{H}_{\mathrm{eff}}(H_+^{\mathrm{gad}},2^n,f(\lambda)) = \frac{-k(-\lambda)^k}{(k-1)!}H^{\mathrm{comp}} \otimes P_+ + O(\lambda^{k+1}), \tag{55}$$

where P_+ acts only on the ancilla registers, projecting them all into the $|+\rangle$ state. Hence, as asserted in Sec. I, the two-local gadget Hamiltonian H^{gad} generates effective interactions which mimic the k-local Hamiltonian H^{comp}.

For a polynomial time adiabatic quantum computation one needs a Hamiltonian that varies smoothly in time and has an eigenvalue gap at worst polynomially small. Let $H(t)$ be a k-local Hamiltonian of this type. For each time t one can construct the corresponding instantaneous gadget Hamiltonian $H^{\mathrm{gad}}(t)$ as described in Sec. I. It is not hard to show that $H^{\mathrm{gad}}(t)$ varies smoothly in time and has a gap that is polynomial in n for any fixed k. Thus $H^{\mathrm{gad}}(t)$ is a 2–local polynomial-time adiabatic algorithm that simulates the original k-local algorithm $H(t)$. In addition to adiabatic quantum computation we expect that kth order gadgets may have many other applications in quantum computation, such as proving QMA-completeness.

IV. NUMERICAL EXAMPLES

In this section we numerically examine the performance of perturbative gadgets in some small examples. As shown in Sec. III, the shifted effective Hamiltonian is that given in Eq. (55). We define

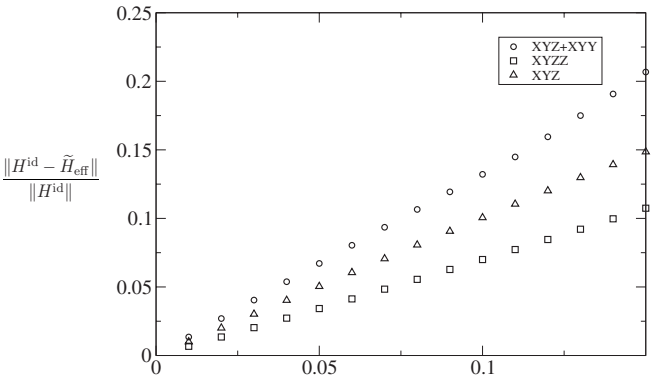

FIG. 2. Here the ratio of the error terms to the ideal Hamiltonian $H^{\mathrm{id}} \equiv \frac{-k(-\lambda)^k}{(k-1)!}H^{\mathrm{comp}}$ is plotted. We examine three examples, a third-order gadget simulating a single XYZ interaction, a third-order gadget simulating a pair of interactions $XYZ+XYY$, and a fourth-order gadget simulating a fourth-order interaction $XYZZ$. Here $\tilde{H}_{\mathrm{eff}}$ is calculated by direct numerical computation without using perturbation theory. As expected the ratio of the norm of the error terms to H^{id} goes linearly to zero with shrinking λ.

$$H^{\mathrm{id}} \equiv \frac{-k(-\lambda)^k}{(k-1)!}H^{\mathrm{comp}} \otimes P_+. \tag{56}$$

$\tilde{H}_{\mathrm{eff}}$ consists of the ideal piece H^{id}, which is of order λ^k, plus an error term of order λ^{k+1} and higher. For sufficiently small λ, these error terms are therefore small compared to the H^{id} term which simulates H^{comp}. Indeed, by a calculation very similar to that which appears in Appendix B, one can easily place an upper bound on the norm of the error terms. However, in practice the actual size of the error terms may be smaller than this bound. To examine the error magnitude in practice, we plot $\frac{\|H^{\mathrm{id}}-\tilde{H}_{\mathrm{eff}}\|}{\|H^{\mathrm{id}}\|}$ in Fig. 2 using direct numerical computation of $\tilde{H}_{\mathrm{eff}}$ without perturbation theory. $f(\lambda)$ was calculated analytically for these examples. In all cases the ratio of $\|H^{\mathrm{id}}-\tilde{H}_{\mathrm{eff}}\|$ to $\|H^{\mathrm{id}}\|$ scales approximately linearly with λ, as one expects since the error terms are of order λ^{k+1} and higher, whereas H^{id} is of order λ^k.

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APPENDIX A: DERIVATION OF PERTURBATIVE FORMULAS

In this appendix we give a self-contained presentation of the derivations for the method of degenerate perturbation theory used in this paper. We closely follow Bloch [4]. Given a Hamiltonian of the form

$$H = H^{(0)} + \lambda V \tag{A1}$$

we wish to find the effective Hamiltonian induced by the perturbation λV on the ground space of $H^{(0)}$. In what follows, we assume that the ground space of $H^{(0)}$ has energy zero. This simplifies notation, and the generalization to nonzero ground energy is straightforward. To further simplify notation we define

$$\hat{V} = \lambda V. \tag{A2}$$

Suppose the ground space of $H^{(0)}$ is d dimensional and denote it by $\mathcal{E}^{(0)}$. Let $|\psi_1\rangle, \ldots, |\psi_d\rangle$ be the perturbed eigenstates arising from the splitting of this degenerate ground space, and let $E_1, \ldots, E_d$ be their energies. Furthermore, let $|\alpha_j\rangle = P_0|\psi_j\rangle$, where P_0 is the projector onto the unperturbed ground space of $H^{(0)}$. If λ is sufficiently small, $|\alpha_1\rangle, \ldots, |\alpha_d\rangle$ are linearly independent, and we can define an operator $\mathcal{U}$ such that

$$\mathcal{U}|\alpha_j\rangle = |\psi_j\rangle \tag{A3}$$

and

$$\mathcal{U}|\phi\rangle = 0 \quad \forall \quad |\phi\rangle \in \mathcal{E}^{(0)\perp}. \tag{A4}$$

Now let $\mathcal{A}$ be the operator

$$\mathcal{A} = P_0 \hat{V} \mathcal{U}. \tag{A5}$$

$\mathcal{A}$ has $|\alpha_1\rangle, \ldots, |\alpha_d\rangle$ as its eigenstates, and $E_1, \ldots, E_d$ as its corresponding energies. To see this, note that since $H^{(0)}$ has zero ground-state energy

$$P_0 \hat{V} = P_0 (H^{(0)} + \hat{V}) = P_0 H. \tag{A6}$$

Thus,

$$\mathcal{A}|\alpha_j\rangle = P_0 \hat{V} \mathcal{U} |\alpha_j\rangle = P_0 \hat{V} |\psi_j\rangle = P_0 H |\psi_j\rangle = P_0 E_j |\psi_j\rangle = E_j |\alpha_j\rangle. \tag{A7}$$

The essential task in this formulation of degenerate perturbation theory is to find a perturbative expansion for $\mathcal{U}$. From $\mathcal{U}$ one can obtain $\mathcal{A}$ by Eq. (A5). By diagonalizing $\mathcal{A}$ one obtains $E_1, \ldots, E_d$, and $|\alpha_1\rangle, \ldots, |\alpha_d\rangle$. Then, by applying $\mathcal{U}$ to $|\alpha_j\rangle$ one obtains $|\psi_j\rangle$. So, given a perturbative formula for $\mathcal{U}$, all quantities of interest can be calculated. Rather than diagonalizing $\mathcal{A}$ to obtain individual eigenstates and eigenenergies, one can instead compute an effective Hamiltonian for the entire perturbed eigenspace, defined by

$$H_{\text{eff}}(H,d) \equiv \sum_{j=1}^{d} E_j |\psi_j\rangle\langle\psi_j|. \tag{A8}$$

This is given by

$$H_{\text{eff}}(H,d) = \mathcal{U}\mathcal{A}\mathcal{U}^{\dagger}. \tag{A9}$$

To derive a perturbative formula for $\mathcal{U}$, we start with Schrödinger's equation

$$H|\psi_j\rangle = E_j|\psi_j\rangle. \tag{A10}$$

By Eq. (A6), left-multiplying this by P_0 yields

$$P_0 \hat{V} |\psi_j\rangle = E_j |\alpha_j\rangle. \tag{A11}$$

By Eq. (A4),

$$\mathcal{U} P_0 = \mathcal{U}. \tag{A12}$$

Thus left-multiplying Eq. (A11) by $\mathcal{U}$ yields

$$\mathcal{U}\hat{V}|\psi_j\rangle = E_j|\psi_j\rangle. \tag{A13}$$

By subtracting (A13) from (A10) we obtain

$$(H - \mathcal{U}\hat{V})|\psi_j\rangle = 0. \tag{A14}$$

The span of $|\psi_j\rangle$ we call $\mathcal{E}$. For any state $|\beta\rangle$ in $\mathcal{E}$ we have

$$(H - \mathcal{U}\hat{V})|\beta\rangle = 0. \tag{A15}$$

Since $\mathcal{U}|\gamma\rangle \in \mathcal{E}$ for any state $|\gamma\rangle$, it follows that

$$(H - \mathcal{U}\hat{V})\mathcal{U} = 0. \tag{A16}$$

This equation can be rewritten as

$$H^{(0)}\mathcal{U} = -\hat{V}\mathcal{U} + \mathcal{U}\hat{V}\mathcal{U}. \tag{A17}$$

Defining $Q_0 = \mathbb{1} - P_0$, we have

$$\mathcal{U} = P_0\mathcal{U} + Q_0\mathcal{U}. \tag{A18}$$

Substituting this into the left-hand side of (A17) yields

$$H^{(0)}Q_0\mathcal{U} = -\hat{V}\mathcal{U} + \mathcal{U}\hat{V}\mathcal{U}, \tag{A19}$$

because $H^{(0)}P_0 = 0$. In $\mathcal{E}^{(0)\perp}$, $H^{(0)}$ has a well-defined inverse and one can write

$$Q_0\mathcal{U} = -\frac{1}{H^{(0)}} Q_0 (\hat{V}\mathcal{U} - \mathcal{U}\hat{V}\mathcal{U}). \tag{A20}$$

Using Eq. (A18), one obtains

$$\mathcal{U} = P_0\mathcal{U} - \frac{1}{H^{(0)}} Q_0 (\hat{V}\mathcal{U} - \mathcal{U}\hat{V}\mathcal{U}). \tag{A21}$$

By the definition of $\mathcal{U}$ it is apparent that $P_0\mathcal{U} = P_0$, thus this equation simplifies to

$$\mathcal{U} = P_0 - \frac{1}{H^{(0)}} Q_0 (\hat{V}\mathcal{U} - \mathcal{U}\hat{V}\mathcal{U}). \tag{A22}$$

We now expand $\mathcal{U}$ in powers of λ (equivalently, in powers of $\hat{V}$), and denote the mth-order term by $\mathcal{U}^{(m)}$. Substituting this expansion into Eq. (A22) and equating terms at each order yields the following recurrence relations:

$$\mathcal{U}^{(0)} = P_0, \tag{A23}$$

$$\mathcal{U}^{(m)} = -\frac{1}{H^{(0)}} Q_0 \left(\hat{V}\mathcal{U}^{(m-1)} - \sum_{p=1}^{m-1} \mathcal{U}^{(p)} \hat{V} \mathcal{U}^{(m-p-1)} \right)$$

$$(m = 1,2,3,\ldots). \tag{A24}$$

Note that the sum over p starts at $p=1$, not $p=0$. This is because

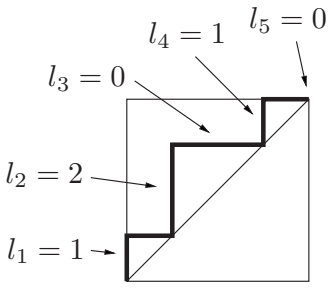

FIG. 3. From a given m-tuple $(l_1, l_2, \ldots, l_m)$ we construct a corresponding stair-step diagram by making the jth step have height l_j, as illustrated.

$$\frac{1}{H^{(0)}} Q_0 \mathcal{U}^{(0)} = \frac{1}{H^{(0)}} Q_0 P_0 = 0. \tag{A25}$$

Let

$$S^l = \begin{cases} \dfrac{1}{(-H^{(0)})^l} Q_0 & \text{if } l > 0, \\ -P_0 & \text{if } l = 0. \end{cases} \tag{A26}$$

$\mathcal{U}^{(m)}$ is of the form

$$\mathcal{U}^{(m)} = \sum{}' S^{l_1} \hat{V} S^{l_2} \hat{V} \cdots S^{l_m} \hat{V} P_0, \tag{A27}$$

where Σ' is a sum over some subset of m-tuples $(l_1, l_2, \ldots, l_m)$ such that

$$l_i \geq 0 \quad (i = 1, 2, \ldots, m), \tag{A28}$$

$$l_1 + l_2 + \cdots + l_m = m. \tag{A29}$$

The proof is an easy induction. $\mathcal{U}^{(0)}$ clearly satisfies this, and we can see that if $\mathcal{U}^{(j)}$ has these properties for all $j < m$, then by recurrence (A24), $\mathcal{U}^{(m)}$ also has these properties.

All that remains is to prove that the subset of allowed m-tuples appearing in the sum Σ' are exactly those which satisfy

$$l_1 + \cdots + l_p \geq p \quad (p = 1, 2, \ldots, m-1). \tag{A30}$$

Following [4], we do this by introducing stair-step diagrams to represent the m-tuples, as shown in Fig. 3.

The m-tuples with property (A30) correspond to diagrams in which the steps lie above the diagonal. Following [4] we call these convex diagrams. Thus, our task is to prove that the sum Σ' is over all and only the convex diagrams. To do this, we consider the ways in which convex diagrams of order m can be constructed from convex diagrams of lower order. We then relate this to the way $\mathcal{U}^{(m)}$ is obtained from lower-order terms in the recurrence (A24).

In any convex diagram, $l_1 \geq 1$. We now consider the two cases $l_1 = 1$ and $l_1 > 1$. In the case that $l_1 = 1$, the diagram is as shown on the left-hand side of Fig. 4.

In any convex diagram of order m with $l_1 = 1$, there is an intersection with the diagonal after one step, at the point that we have labeled c. The diagram from c to b is a convex diagram of order $m-1$. Conversely, given any convex diagram of order $m-1$ we can construct a convex diagram of order m by adding one step to the beginning. Thus, the convex diagrams of order m with $l_1 = 1$ correspond bijectively to the convex diagrams of order $m-1$.

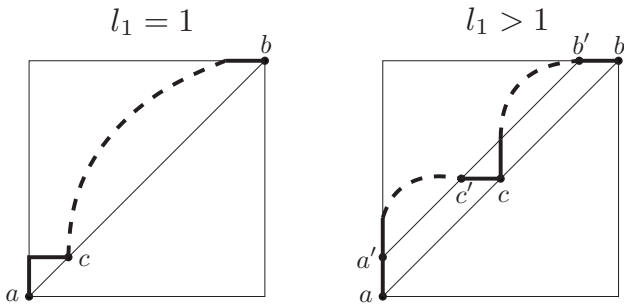

FIG. 4. A convex diagram must have either $l_1 = 1$ or $l_1 > 1$. In either case, the diagram can be decomposed as a concatenation of lower-order convex diagrams.

The case $l_1 > 1$ is shown in Fig. 4 on the right-hand side. Here we introduce the line from a' to b', which is parallel to the diagonal, but higher by one step. Since the diagram must end at b, it must cross back under $a'b'$ at some point. We label the first point at which it does so as c'. In general, c' can equal b'. The curve going from a' to c' is a convex diagram of order p with $1 \leq p \leq m-1$, and the curve going from c to b is a convex diagram of order $n-p-1$ (which may be order zero if $c' = b'$). Since c' exists and is unique, this establishes a bijection between the convex diagrams of order m with $l_1 > 1$, and the set of the pairs of convex diagrams of orders p and $n-p-1$, for $1 \leq p \leq n-1$.

Examining the recurrence (A24), we see that the $l_1 = 1$ diagrams are exactly those which arise from the term

$$\frac{Q_0}{H^{(0)}} \hat{V} \mathcal{U}^{(m-1)} \tag{A31}$$

and the $l_1 > 1$ diagrams are exactly those which arise from the term

$$\frac{Q_0}{H^{(0)}} \sum_{p=1}^{m-1} \mathcal{U}^{(p)} \hat{V} \mathcal{U}^{(n-p-1)}. \tag{A32}$$

which completes the proof that Σ' is over the m-tuples satisfying Eq. (A30).

APPENDIX B: CONVERGENCE OF PERTURBATION SERIES

Here we show that the perturbative expansion for $\mathcal{U}$ given in Eq. (27) converges for

$$\|\lambda V\| < \frac{\gamma}{4}. \tag{B1}$$

By Eq. (20), the convergence of $\mathcal{U}$ also implies the convergence of $\mathcal{A}$. Applying the triangle inequality to Eq. (27) yields

$$\|\mathcal{U}\| \leq 1 + \sum_{m=1}^{\infty} \|\mathcal{U}^{(m)}\|. \tag{B2}$$

Substituting in Eq. (28) and applying the triangle inequality again yields

$$\|\mathcal{U}\| \leq 1 + \sum_{m=1}^{\infty} \lambda^m \sum_{(m)} \|S^{l_1} \cdots V S^{l_m} V P_0\|. \tag{B3}$$

By the submultiplicative property of the operator norm,

$$\|\mathcal{U}\| \leq 1 + \sum_{m=1}^{\infty} \lambda^m \sum_{(m)} \|S^{l_1}\| \times \|V\| \times \ldots \times \|V\| \times \|S^{l_m}\| \times \|V\| \times \|P_0\|. \tag{B4}$$

$\|P_0\| = 1$, and by Eq. (22) we have

$$\|S^l\| = \frac{1}{(E_1^{(0)})^l} = \frac{1}{\gamma^l}. \tag{B5}$$

Since the sum in Eq. (B4) is over $l_1 + \cdots + l_m = m$, we have

$$\|\mathcal{U}\| \leq 1 + \sum_{m=1}^{\infty} \sum_{(m)} \frac{\|\lambda V\|^m}{\gamma^m}. \tag{B6}$$

The sum $\Sigma_{(m)}$ is over a subset of the m-tuples adding up to m. Thus, the number of terms in this sum is less than the number of ways of obtaining m as a sum of m non-negative integers. By elementary combinatorics, the number of ways to obtain n as a sum of r non-negative integers is $\binom{n+r-1}{n}$, thus

$$\|\mathcal{U}\| \leq 1 + \sum_{m=1}^{\infty} \binom{2m-1}{m} \frac{\|\lambda V\|^m}{\gamma^m}. \tag{B7}$$

Since

$$\sum_{j=0}^{2m-3} \binom{2m-1}{j} = 2^{2m-1}, \tag{B8}$$

we have

$$\binom{2m-1}{m} \leq 2^{2m-1}. \tag{B9}$$

Substituting this into Eq. (B7) converts it into a convenient geometric series

$$\|\mathcal{U}\| \leq 1 + \sum_{m=1}^{\infty} 2^{2m-1} \frac{\|\lambda V\|^m}{\gamma^m}. \tag{B10}$$

This series converges for

$$\frac{4\|\lambda V\|}{\gamma} < 1. \tag{B11}$$

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