Quadratization in Discrete Optimization and Quantum Mechanics

Richard Tanburn,[1,*] Nicholas Chancellor,[2,†] and Nike Dattani[1,3,4,‡]

[1]*Oxford University, Department of Mathematics*
[2]*Durham University, Department of Physics*
[3]*McMaster University, Department of Chemistry and Chemical Biology*
[4]*Harvard-Smithsonian Center for Astrophysics*

A collaborative, evolving, open review paper on k-local to 2-local transformations (quadratizations) in classical computing, quantum annealing, and universal adiabatic quantum computing.

When optimizing discrete functions, it is often easier when the function is qudaratic than if it is of higher degree. But notice that the cubic and quadratic funcitons:

$$b_1 b_2 + b_2 b_3 + b_3 b_4 - 4 b_1 b_2 b_3 \quad \text{(cubic)}, \tag{1}$$
$$b_1 b_2 + b_2 b_3 + b_3 b_4 + 4 b_1 - 4 b_1 b_2 - 4 b_1 b_3 \quad \text{(quadratic)}, \tag{2}$$

where each b_i can either be 0 or 1, both never go below the value of -1, and all minima have the form $(b_1, b_2, b_3, b_4) = (1, 1, 1, b_4)$. Therefore if we are interested in the ground state of a discrete function of degree k, we may optimize either function and get exactly the same result. **Part I** gives more than 15 different ways to do this.

The binary variables b_i can be either of the eigenvalues of the matrix b below, which is related to the Pauli z matrix by $z = 2b - \mathbb{1}$. Other Pauli matrices are listed below:

$$b \equiv \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \ z \equiv \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \ x \equiv \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \ y \equiv \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}, \ \mathbb{1} \equiv \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \tag{3}$$

Any Hermitian 2×2 matrix can be written as a linear combination of the Pauli matrices $z, x, y, \mathbb{1}$, so we can therefore describe the Hamiltonian of any number of spin-$^1/_2$ particles by a function of Pauli matrices acting on each particle, for instance:

$$z_1 x_2 + x_2 y_3 + z_3 z_4 - 4 y_1 y_2 z_3 \quad \text{(cubic)}, \tag{4}$$

where the coefficients tell us about the strengths of couplings between these particles. The Schrödinger equation tells us that the eigenvalues of the Hamiltonian are the allowed energy levels and their eigenvectors (wavefunctions) are the corresponding physical states. More generally these do not have to be spins but can be any type of qubits, and we can encode the solution to *any* problem in the ground state of a Hamiltonian, then solve the problem by finding the lowest energy state of the physical system (this is called adiabatic quantum computing).

Two-body physical interactions occur more naturally than many-body interactions so **Parts II-III** give more than 10 different ways to quadratize genreal Hamiltonians (some of these methods do not even require the s_i to be 2×2 matrices, meaning that we can have types of qudits that are not qubits).

The optimization problems of Eqs. (1)-(2) are specific cases of the type in Eq. (4) where only z matrices are present.

Part I

Diagonal Hamiltonians (pseudo-Boolean functions)

I. METHODS THAT INTRODUCE ZERO AUXILIARY VARIABLES

A. Deduction Reduction (Deduc-reduc)

Summary
We look for *deductions* (e.g. $b_1 b_2 = 0$) that must hold true at the global minimum. These can be found by *a priori* knowledge of the given problem, or by enumerating solutions of a small subset of the variables. We can then substitute high-order terms using the low-order terms of the deduction, and add on a penalty term to preserve the ground states [1].

Cost
- 0 auxiliary variables needed.

- For a particular value of m, we have $\binom{n}{m}$ different m-variable subsets of the n variable problem, and $\binom{n}{m}2^m$ evaluations of the objective function to find all possible m-variable deductions, whereas 2^n evaluations is enough to solve the entire problem. We therefore choose $m \lll n$.

Pros
- No auxiliary variables needed.

Cons
- When deductions cannot be determined naturally (as in the Ramsey number determination problem, see Example IX), deductions need to be found by 'brute force', which scales exponentially with respect to m. For highly connected systems (systems with a large number of non-zero α_{ij} coefficients), the value of m required to find even one deduction can be prohibitively large.

Example
Consider the Hamiltonian:

$$H_{4-\text{local}} = b_1 b_2 (10 + b_3 + b_3 b_4) + b_1(b_3 - 3) + b_2(b_3 - 2b_3 - b_4 - 1) + F(x_3, x_4, x_5, \ldots, x_N) \quad (5)$$

where F is any polynomial in b_i for $i \geq 3$.
Since the coefficient of $b_1 b_2$ is 10, which is greater than the sum of all of the other coefficients involving b_1 or b_2, ***it must be the case that*** $b_1 b_2 = 0$. Specifically, for the 4 assignments of (b_3, b_4), we see that $b_1 b_2 = 0$ at every minimum of $H_{4-\text{local}} - F$.
Using deduc-reduc we have:

$$H_{2-\text{local}} = 12 b_1 b_2 + b_1(b_3 - 3) + b_2(b_3 - 2b_3 - b_4 - 1) + F(x_3, x_4, x_5, \ldots, x_N) \quad (6)$$

which has the same global minima as $H_{4-\text{local}}$ but one fewer quartic and one fewer cubic term.

Bibliography
- Original paper, with more implementation details, and application to integer factorization: [1].

B.   ELC Reduction

Summary
An Excludable Local Configuration (ELC) is a partial assignment of variables that make it impossible to achieve the minimum. We can therefore add a term that corresponds to the energy of this ELC without changing the solution to the minimization problem. In practice we can eliminate all monomials with a variable in which a variable is set to 0, and reduce any variable set to 1. Given a general Hamiltonian we can try to find ELCs by enumerating solutions of a small subset of variables in the problem [2].

Cost
- 0 auxiliary variables needed.

- For a particular value of m, we have $\binom{n}{m}$ different m-variable subsets of the n variable problem, and $\binom{n}{m}2^m$ evaluations of the objective function to find all possible m-variable deductions, whereas 2^n evaluations is enough to solve the entire problem. We therefore choose $m \lll n$.

- Approximate methods exist which have been shown to be much faster and give good approximations to the global minimum [2].

Pros
- No auxiliary variables needed.

Cons
- No known way to find ELCs except by 'brute force', which scales exponentially with respect to m.

- ELCs do not always exist.

Example
Consider the Hamiltonian:

$$H_{3-\text{local}} = b_1 b_2 + b_2 b_3 + b_3 b_4 - 4 b_1 b_2 b_3. \tag{7}$$

If $b_1 b_2 b_3 = 0$, no assignment of our variables will we be able to reach a lower energy than if $b_1 b_2 b_3 = 1$. Hence this gives us *twelve* ELCs, and one example is $(b_1, b_2, b_3) = (1, 0, 0)$ which we can use to form the polynomial:

$$H_{2-\text{local}} = H_{3-\text{local}} + 4 b_1 (1 - b_2)(1 - b_3) \tag{8}$$
$$= b_1 b_2 + b_2 b_3 + b_3 b_4 + 4 b_1 - 4 b_1 b_2 - 4 b_1 b_3. \tag{9}$$

In both cases Eqs. (7) and (9), the only global minima occur when $b_1 b_2 b_3 = 1$.

Bibliography
- Original paper and application to computerized image denoising: [2].

C.   Groebner Bases

Summary
Given a set of polynomials, a Groebner basis is another set of polynomials that have exactly the same zeros. The advantage of a Groebner basis is it has nicer algebraic properties than the original equations, in particular they tend to have smaller degree polynomials. The algorithms for calculating Groebner bases are generalizations of Euclid's algorithm for the polynomial greatest common divisor.

Work has been done in the field of 'Boolean Groebner bases', but while the variables are Boolean the coefficients of the functions are in $\mathbb{F}_2$ rather than $\mathbb{Q}$.

Cost
- 0 auxiliary variables needed.

- $\mathcal{O}\left(2^{2^n}\right)$ in general, $\mathcal{O}(d^{n^2})$ if the zeros of the equations form a set of discrete points, where d is the degree of the polynomial and n is the number of variables [3].

Pros
- No auxiliary variables needed.

- General method, which can be used for other rings, fields or types of variables.

Cons
- Best algorithms for finding Groebner bases scale double exponentially in n.

- Only works for Hamiltonians whose minimization corresponds to solving systems of discrete equations, as the method only preserves roots, not minima.

Example
Consider the following pair of equations:

$$b_1 b_2 b_3 b_4 + b_1 b_3 + b_2 b_4 - b_3 = b_1 + b_1 b_2 + b_3 - 2 = 0. \tag{10}$$

Feeding these to Mathematica's `GroebnerBasis` function, along with the binarizing $b_1(b_1 - 1) = \ldots = b_4(b_4 - 1) = 0$ constraints, gives a Groebner basis:

$$\{b_4 b_3 - b_4, b_2 + b_3 - 1, b_1 - 1\}. \tag{11}$$

From this we can immediately read off the solutions $b_1 = 1$, $b_2 = 1 - b_3$ and reduce the problem to $b_3 b_4 - b_4 = 0$. Solving this gives a final solution set of: $(b_1, b_2, b_3, b_4) = (1, 0, 1, 0), (1, 0, 1, 1), (1, 1, 0, 0)$, which should be the same as the original 4-local problem.

Bibliography
- Reduction and embedding of factorizations of all bi-primes less than $200,000$: [4].

D.   Split Reduction

Summary

It has been shown in [5] that, if multiple runs of a minimization algorithm is permitted, it is possible to reduce a lot of the problem by conditioning on the most connected variables. We call each of these operations a *split*.

Cost

Exponential in the number of splits, as the number of problems to solve doubles with every split.

Pros
- This method can be applied to any problem and can be very effective on problems with a few very connected variables.

Cons
- Exponential cost in the worst case.

Example

Consider the simple objective function

$$H = 1 + b_1 b_2 b_5 + b_1 b_6 b_7 b_8 + b_3 b_4 b_8 - b_1 b_3 b_4. \tag{12}$$

In order to quadratize H, we first have to choose a variable to split over. In this case b_1 is the obvious choice since it is present in the most terms and contributes to the quartic term. We then obtain two different problems:

$$H_0 = 1 + b_3 b_4 b_8 \tag{13}$$
$$H_1 = 1 + b_2 b_5 + b_6 b_7 b_8 + b_3 b_4 b_8 - b_3 b_4. \tag{14}$$

At this point, we could split H_0 again and solve it entirely, or use a variable we saved in the previous split to quadratize our only problem.

To solve H_1, we can split again on b_8, resulting in problems:

$$H_{1,0} = 1 + b_2 b_5 + b_6 b_7 \tag{15}$$
$$H_{1,1} = 1 + b_2 b_5 + b_3 b_4. \tag{16}$$

Now both of these problems are quadratic. Hence we have reduced our original, hard problem into 3 easy problems, requiring only 2 extra (much easier) runs of our minimization algorithm, and without needing any auxiliary variables.

Bibliography
- Original paper and application to Ramsey number determination: [5].

II. METHODS THAT INTRODUCE AUXILIARY VARIABLES TO QUADRATIZE A SINGLE TERM

A. Negative Term Reduction

Summary

For a negative term $-b_1 b_2 ... b_k$, introduce a single auxiliary variable b_a and make the substitution:

$$- b_1 b_2 \ldots b_k = \min_{b_a} \left((k - 1 - \sum_i b_i) b_a \right). \tag{17}$$

Cost
- 1 auxiliary variable for each k-local term.

Pros
- All resulting quadratic terms are submodular (have negative coefficients).

- Can reduce arbitrary order terms with only 1 auxiliary.

Cons
- Only works for negative terms.

Example

$$H_{6-\mathrm{local}} = -2 b_1 b_2 b_3 b_4 b_5 b_6 + b_5 b_6, \tag{18}$$

has a unique minimum energy of -1 when all $b_i = 1$.

$$H_{2-\mathrm{local}} = 2 \left(5 b_a - b_1 b_a - b_2 b_a - b_3 b_a - b_4 b_a - b_5 b_a - b_6 b_a \right) + b_5 b_6 \tag{19}$$

has the same unique minimum energy, and it occurs at the same place (all $b_i = 1$), with $b_a = 1$.

Bibliography
- 2004: Kolmogorov and Zabih presented this for cubic terms [6].

- 2005: Generalized to arbitrary order by Freedman and Drineas [7].

- Discussion: [8], [9].

B.   Gruber Positive Term Reduction

Summary

Suppose we have a monomial $b_1 b_2 b_3 \ldots b_k$ with $k > 2$. Let $X = \sum_{i=1}^{k} b_i$.

Let $m = \lceil \frac{k}{4} \rceil$, $N = n - 2m$ and $Y = \sum_{j=2}^{m} b'_j$ where $b'_1, \ldots, b'_m$ are auxiliary variables. Note that the j index starts at 2. Then:

$$b_1 \ldots b_k = \min_{b'_1, \ldots b'_m} \frac{1}{2} \left(X - N b'_1 - 2Y \right) \left(X - N b'_1 - 2Y - 1 \right) \tag{20}$$

Cost

$\lceil \frac{k}{4} \rceil$ auxiliary qubits per positive monomial.

Pros

- Smallest number of auxiliary coefficients that scales linearly with k.

- Smaller coefficients than the logarithmic reduction.

Cons

- Introduces many non-submodular terms.

Example

Consider $k = 4$, so that $m = 1$, $N = 2$. Then:

$$b_1 b_2 b_3 b_4 = \min_{b'} \frac{1}{2} \left(b_1 + b_2 + b_3 + b_4 - 2b'_1 \right) \left(b_1 + b_2 + b_3 + b_4 - 2b'_1 - 1 \right) \tag{21}$$

Bibliography

- Original paper: [19].

C. Logarithmic Positive Monomial Reduction

Summary
Suppose we have a monomial $b_1 b_2 b_3 \ldots b_k$. Pick n minimal such that $k < 2^{n+1}$ and let $N = 2^{n+1} - k$.
For convenience, let $X = \sum_{i=1}^{k} b_i$.

$$b_1 \ldots b_k = \min_{b_1', \ldots b_n'} \frac{1}{2} \left(N + X - \sum_{i=1}^{n} 2^i b_i' \right) \left(N + X - \sum_{i=1}^{n} 2^i b_i' - 1 \right) \tag{22}$$

Cost
$\lceil \log k \rceil - 1$ auxiliary qubits per positive monomial.

Pros
- Logarithmic number of auxiliary variables.

Cons
- Introduces many non-submodular terms.

Example
Consider $k = 4$, so that $n = 2$, $N = 4$. Then:

$$b_1 b_2 b_3 b_4 = \min_{b_1', b_2'} \frac{1}{2} \left(4 + b_1 + b_2 + b_3 + b_4 - b_1' - 2b_2' \right) \left(3 + b_1 + b_2 + b_3 + b_4 - b_1' - 2b_2' \right) \tag{23}$$

Bibliography
- Original paper: [19].

D. Positive Term Reduction

Summary

By considering the negated literals $\bar{b}_i = 1 - b_i$, we recursively apply the previous method to $b_1 b_2 \ldots b_k = -\bar{b}_1 b_2 \ldots b_k + b_2 b_3 \ldots b_k$. The final identity is:

$$b_1 b_2 \ldots b_k = \min_{b_a} \left(\sum_{i=1}^{k-2} b_{a_i} \left(k - i - 1 + b_i - \sum_{j=i+1}^{k} b_j \right) \right) + b_{k-1} b_k \tag{24}$$

Cost
- $k - 2$ auxiliary variables for each k-local term.

Pros
- Works for positive monomials.

Cons
- $k - 1$ non-submodular quadratic terms.

Example

$$b_1 b_2 b_3 b_4 = \min_{b_a} b_{a_1} \left(2 + b_1 - b_2 - b_3 - b_4 \right) + b_{a_2} \left(1 + b_2 - b_3 - b_4 \right) + b_3 b_4 \tag{25}$$

Bibliography
- Summary: [10].

E. Ishikawa's Symmetric Reduction (Positive Term Reduction)

Summary

This method re-writes a positive monomial using symmetric polynomials, so all possible quadratic terms are produced and they are all non-submodular:

$$b_1...b_k = \min_{b_{a_1},...,b_{a_{n_k}}} \left(\sum_{i=1}^{n_k} b_{a_i} \left(c_{i,d} \left(-\sum_{j=1}^{k} b_j + 2i \right) - 1 \right) + \sum_{i<j} b_i b_j \right) \qquad (26)$$

where $n_k = \left\lfloor \frac{k-1}{2} \right\rfloor$ and $c_{i,k} = \begin{cases} 1, & i = n_d \text{ and } k \text{ is odd}, \\ 2, & \text{else}. \end{cases}$

Cost
- $\left\lfloor \frac{k-1}{2} \right\rfloor$ auxiliary variables for each k-order term

- $\mathcal{O}(kt)$ for a k-local Hamiltonian with t terms.

Pros
- Works for positive monomials. About half as many auxiliary variables for each k-order term as the previous method.

Cons
- $\mathcal{O}(k^2)$ quadratic terms are created, which may make chimerization more costly.

- $\frac{k(k-1)}{2}$ non-submodular terms.

- Worse than the previous method for quartics, with respect to submodularity.

Example

$$b_1 b_2 b_3 b_4 = \min_{b_a}(3 - 2b_1 - 2b_2 - 2b_3 - 2b_4)b_a + b_1 b_2 + b_1 b_3 + b_1 b_4 + b_2 b_3 + b_2 b_4 + b_3 b_4 \qquad (27)$$

Bibliography
- Original paper and application to image denoising: [8].

F.   Reduction by Minimum Selection (Kolmogorov & Zabih, 2004)

Summary

This method can be used to re-write positive or negative cubic terms in terms of 6 quadratic terms. The identity is given by:

$$b_1 b_2 b_3 \rightarrow 1 - (b_a + b_1 + b_2 + b_3) + b_a (b_1 + b_2 + b_3) + b_1 b_2 + b_1 b_3 + b_2 b_3 \tag{28}$$

Cost
- 1 auxiliary variable per positive or negative cubic term.

Pros
- Works on positive or negative monomials.

- Reproduces the full spectrum.

Cons
- Introduces all 6 possible non-submodular quadratic terms.

Bibliography
- Original paper: [6].

G. Reduction by Minimum Selection (in terms of z)

Summary

The formula is almost the same as in the version in terms of b, but with a factor of 2, a change of sign for the linear terms, and a slight change in the constant term:

$$\pm z_1 z_2 z_3 = 3 \pm \left(z_1 + z_2 + z_3 + z_a \right) + 2 z_a \left(z_1 + z_2 + z_3 \right) + z_1 z_2 + z_1 z_3 + z_2 z_3. \tag{29}$$

Cost
- 1 auxiliary variable per positive or negative cubic term.

Pros
- Works on positive or negative monomials.

- Reproduces the full spectrum.

Cons
- Introduces all 6 possible non-submodular quadratic terms.

Bibliography
- 31 March 2016 published by Chancellor, Zohren, and Warburton without the constant term: [11].

- 8 April 2016 published independently by Leib, Zoller, and Lechner without the constant term [12, 13].

H.   Asymmetric Reduction

Summary
Similar to other methods of reducing one term, this method can reduce a positive cubic monomial into quadratic terms using only one auxiliary variable, while introducing fewer non-submodular terms than the symmetric version.
The identity is given by:

$$b_1 b_2 b_3 = \min_{b_a} \left(b_a - b_2 b_a - b_3 b_a + b_1 b_a + b_2 b_3 \right) \tag{30}$$

$$= \min_{b_a} \left(b_a - b_1 b_a - b_3 b_a + b_2 b_a + b_1 b_3 \right) \tag{31}$$

$$= \min_{b_a} \left(b_a - b_1 b_a - b_2 b_a + b_3 b_a + b_1 b_2 \right). \tag{32}$$

$$\tag{33}$$

Cost
1 auxiliary variable per positive cubic term.

Pros
• Works on positive monomials.

• Fewer non-submodular terms than Ishikawa Reduction.

Cons
• Only been shown to work for cubics.

Example

$$b_1 b_2 b_3 + b_1 b_3 - b_2 = \min_{b_a} \left(b_a - b_1 b_a - b_3 b_a + b_2 b_a + 2 b_1 b_3 \right) - b_2 \tag{34}$$

Bibliography
• Original paper and application to computer vision: [14].

I. Bit flipping

Summary
For any variable b, we can consider the negation $\bar{b} = 1 - b$. The process of exchanging b for $\bar{b}$ is called *flipping*. Using bit-flipping, an arbitrary function in n variables can be represented using at most $2^{(n-2)}(n - 3) + 1$ variables, though this is a gross overestimate.
Can be used in many different ways:

1. Flipping positive terms and using II A, recursively;

2. For $\alpha < 0$, we can reduce $\alpha \bar{b}_1 \bar{b}_2 ... \bar{b}_k$ very efficiently to submodular form using II A. A generalized version exists for arbitrary combinations of flips in the monomial which makes reduction entirely submodular [8];

3. When we have quadratized we can minimize the number of non-submodular terms by flipping.

4. We can make use of both b_i and $\bar{b}_i$ in the same Hamiltonian by adding on a sufficiently large penalty term: $\lambda(b_i + \bar{b}_i - 1)^2 = \lambda(1 + 2b_i\bar{b}_i - b_i - \bar{b}_i)$. This is similar to the ideas in reduction by substitution or deduc-reduc. In this way, given a quadratic in n variables we can make sure it only has at most n nonsubmodular terms if we are willing to use the extra n negation variables as well (so we have $2n$ variables in total).

Cost
- None, as replacing b_i with it's negation $\bar{b}_i$ costs nothing except a trivial symbolic expansion.

Pros
- Cheap and effective way of improving submodularity.

- Can be used to combine terms in clever ways, making other methods more efficient.

Cons
- Unless the form of the Hamiltonian is known, spotting these 'factorizations' using negations is difficult.

- We need an auxiliary variable for each b_i for which we also want to use $\bar{b}_i$ in the same Hamiltonian.

Example
By bit-flipping b_2 and b_4, i.e. substituting $b_2 = 1 - \bar{b}_2$ and $b_4 = 1 - \bar{b}_4$, we see that:

$$H = 3b_1b_2 + b_2b_3 + 2b_1b_4 - 4b_2b_4 \tag{35}$$
$$= -3b_1\bar{b}_2 - \bar{b}_2b_3 - 2b_1\bar{b}_4 - \bar{b}_2\bar{b}_4 + 5b_1 + b_3 + 4\bar{b}_2 + 4\bar{b}_4 - 4. \tag{36}$$

The first expression is highly non-submodular while the second is entirely submodular.

Bibliography
- Original paper: [8].

J. Symmetry Based Mappings

Summary

Auxilliary qubits can be made to "count" the number of logical qubits in the 1 configuration. By applying single qubit terms to the auxilliary qubits, the spectrum of *any* permutation symmetric Hamiltonian can be reproduced.

Cost
- For a k local coupler requires k auxilliary qubits.

Pros
- Natural flux qubit implementation [15].

- Single gadget can reproduce any permutation symmetric spectrum.

- High degree of symmetry means this method is natural for some kinds of quantum simulations [16].

Cons
- Requires coupling between all logical bits and from all logical bits to all auxilliary bits.

- Requires single body terms of increasing strength as k is increased.

Example

A 4 qubit gadget guarantees that the number of auxillary bits in the -1 state is equal to the number of logical bits in the 1 state

$$H_{4-\text{count}} = 4 \sum_{i=2}^{4} \sum_{j=1}^{i-1} b_i b_j + 4 \sum_{i=1}^{4} \sum_{j=1}^{4} b_i b_{a_j} - 15 \sum_{i=1}^{4} b_i - 8 \sum_{i=1}^{4} b_{a_i} + \left(5\, b_{a_1} + b_{a_2} - 3\, b_{a_3} - 7\, b_{a_4} \right) + 26 \quad (37)$$

This gadget can be expressed more naturally in terms of z:

$$H_{4-\text{count}} = \sum_{i=2}^{4} \sum_{j=1}^{i-1} z_i z_j - \frac{1}{2} \sum_{i=1}^{4} z_i + \sum_{i=1}^{4} \sum_{j=1}^{4} z_i z_{a_j} + \frac{1}{2} \left(5 z_{a_1} + z_{a_2} - 3\, z_{a_3} - 7 z_{a_4} \right). \quad (38)$$

To replicate the spectrum of $b_1 b_2 b_3 b_4$, we add

$$H_{2-\text{local}} = -b_{a_4} + \lambda H_{4-\text{count}}. \quad (39)$$

where λ is a large number.

For the spectrum of

$$z_1 z_2 z_3 z_4 = 16\, b_1 b_2 b_3 b_4 - 8 \left(b_1 b_2 b_3 + b_1 b_2 b_4 + b_1 b_3 b_4 + b_2 b_3 b_4 \right) +$$
$$4 \left(b_1 b_2 + b_1 b_3 + b_1 b_4 + b_2 b_3 + b_2 b_4 + b_3 b_4 \right) - 2 \left(b_1 + b_2 + b_3 + b_4 \right) + 1, \quad (40)$$

we implement,

$$H_{2-\text{local}} = 2\, b_{a_1} - 2\, b_{a_2} + 2\, b_{a_3} - 2\, b_{a_4} + \lambda H_{4-\text{count}}, \quad (41)$$

Bibliography
- Paper on flux qubit implementation: [15]

- Paper on max-k-sat mapping: [17]

- Talk including use in quantum simulation: [16]

K. Another Cubic Reduction

Summary

$$-b_1 b_2 b_3 = \min_{b_a} b_a \left(-b_1 + b_2 + b_3\right) - b_1 b_2 - b_1 b_3 + b_1 \tag{42}$$

Cost
1 auxiliary variable per negative cubic term.

Pros
- Asymmetric which allows more flexibility in cancelling with other quadratics.

Cons
- Only works for negative cubic monomials.

Example

$$-b_1 b_2 b_3 + b_1 b_3 - b_2 = \min_{b_a} \left(b_a - b_1 b_a - b_3 b_a + b_2 b_a + 2 b_1 b_3\right) - b_2 \tag{43}$$

Bibliography
- Discussion: [8], [18].

III.   METHODS THAT INTRODUCE AUXILIARY VARIABLES TO QUADRATIZE MULTIPLE TERMS WITH THE SAME AUXILIARIES

A.   Reduction by Substitution

Summary

Pick a variable pair (b_i, b_j) and substitute $b_i b_j$ with a new auxiliary variable $b_{a_{ij}}$. Enforce equality in the ground states by adding some scalar multiple of the penalty $P = b_i b_j - 2b_i b_{a_{ij}} - 2b_i b_{a_{ij}} + 3b_{a_{ij}}$ or similar. Since $P > 0$ if and only if $b_{a_{ij}} \neq b_i b_j$, the minimum of the new $(k-1)$-local function will satisfy $b_{a_{ij}} = b_i b_j$), which means that at the minimum, we have precisely the original function. Repeat $(k-2)$ times for each k-local term and the resulting function will be 2-local.

Cost
- 1 auxiliary variable per reduction.

- At most $k\,t$ auxiliary variables for a k-local Hamiltonian of t terms, but usually fewer.

Pros
- Variable can be used across the entire Hamiltonian, reducing many terms at once.

- Very easy to implement.

- Reproduces not only the ground state, but the full spectrum.

Cons
- Inefficient for single terms as it introduces many auxiliary variables compared to Ishikawa reduction, for example.

- Introduces quadratic terms with large positive coefficients, making them highly non-submodular.

- Determining optimal substitutions can be expensive.

Example

We pick the pair (b_1, b_2) and combine.

$$b_1 b_2 b_3 + b_1 b_2 b_4 \mapsto b_3 b_a + b_4 b_a + b_1 b_2 - 2b_1 b_a - 2b_1 b_a + 3b_a \qquad (44)$$

Bibliography
- Original paper: [20]

- Re-discovered in the context of diagonal quantum Hamiltonians: [21].

- Used in: [22, 23].

B. FGBZ Reduction (Fix-Gruber-Boros-Zabih)

Summary
Here we consider a set C of variables which occur in multiple monomials throughout the Hamiltonian. Each application 'rips out' this common component from each term [24][10].

Let $\mathcal{H}$ be a set of monomials, where $C \subseteq H$ for each $H \in \mathcal{H}$ and each monomial H has a weight α_H. The algorithm comes in 2 parts: when all $\alpha_H > 0$ and when all $\alpha_H < 0$. Combining the 2 gives the final method:

1. $\alpha_H > 0$

$$\sum_{H \in \mathcal{H}} \alpha_H \prod_{j \in H} b_j = \min_{b_a} \left(\sum_{H \in \mathcal{H}} \alpha_H \right) b_a \prod_{j \in C} b_j + \sum_{H \in \mathcal{H}} \alpha_H (1 - b_a) \prod_{j \in H \smallsetminus C} b_j \qquad (45)$$

2. $\alpha_H < 0$

$$\sum_{H \in \mathcal{H}} \alpha_H \prod_{j \in H} b_j = \min_{b_a} \sum_{H \in \mathcal{H}} \alpha_H \left(1 - \prod_{j \in C} b_j - \prod_{j \in H \smallsetminus C} b_j \right) b_a \qquad (46)$$

Cost
- One auxiliary variable per application.

- In combination with II A, it can be used to make an algorithm which can reduce t positive monomials of degree d in n variables using $n + t(d-1)$ auxiliary variables in the worst case.

Pros
- Can reduce the connectivity of a Hamiltonian, as it breaks interactions between variables.

Cons
- $\alpha_H > 0$ method converts positive terms into negative ones of same order rather than reducing them, though these can then be reduced more easily.

- $\alpha_H < 0$ method only works for $|C| > 1$, and cannot quadratize cubic terms.

Example
First let $C = b_1$ and use the positive weight version:

$$b_1 b_2 b_3 + b_1 b_2 b_4 \mapsto 2b_{a_1} b_1 + (1 - b_{a_1}) b_2 b_3 + (1 - b_{a_1}) b_2 b_4 \qquad (47)$$
$$= 2b_{a_1} b_1 + b_2 b_3 + b_2 b_4 - b_{a_1} b_2 b_3 - b_{a_1} b_2 b_4 \qquad (48)$$

now we can use II A:

$$-b_{a_1} b_2 b_3 - b_{a_1} b_2 b_4 \mapsto 2b_{a_2} - b_{a_1} b_{a_2} - b_{a_2} b_2 - b_{a_2} b_3 + 2b_{a_2} - b_{a_1} b_{a_2} - b_{a_2} b_2 - b_{a_2} b_4 \qquad (49)$$
$$= 4b_{a_2} - 2b_{a_1} b_{a_2} - 2b_{a_2} b_2 - b_{a_2} b_3 - b_{a_2} b_4. \qquad (50)$$

Bibliography
- Original paper and application to image denoising: [24].

C.   Flag Based SAT Mapping

Summary
This method uses gadgets to produce separate 3-SAT clauses which allow variables which 'flag' the state of pairs of other variables.

Cost
  • Varies, but generally higher than other methods.

Pros
  • Highly general and therefore conducive to proofs.

Cons
  • Designed for generality rather than efficiency.

Example
To create a system which maps $b_1 b_2 b_3$, we use the following gadget (note that this is given in terms of z in the orginal work and translated to b here):

$$H_{3\text{–SAT}}(b_1, b_2, b_3) = 2\sum_{i=1}^{3} b_i b_{a_i} + 2\sum_{i<j}^{3} b_{a_i} b_{a_j} - 4\sum_{i=1}^{3} b_{a_i} - 2\sum_{i=1}^{3} b_i + \frac{23}{2}. \tag{51}$$

Implementing $\lambda H_{3\text{–SAT}}$, creates a situation where b_3 is a 'flag' for b_1 and b_2 in other words b_3 is constrained to be 1 in the low energy manifold if $b_1 = 0$ and $b_2 = 0$. It follows from the universality of $3 - \text{SAT}$ that these 'flag' clauses can be combined to map any spin Hamiltonian. To do this, we also need anti-ferromagnetic couplings to express the 'negated' variable, to do this, we define,

$$H_{\text{AF}}(b_1, b_{\neg 1}) = 2\, b_1 b_{\neg 1} - b_i - b_{\neg 1} + 1. \tag{52}$$

As an explicit example, consider reproducing the spectrum of $z_1 z_2 z_3 = (2\, b_1 - 1)(2\, b_2 - 1)(2\, b_3 - 1)$. In this case we need to assign a higher energy to the $(1, 1, 1)$, $(0, 0, 1)$, $(0, 1, 0)$, and $(1, 0, 0)$ states. A flag (b_f) which is forced into a higher energy state if these conditions are satisfied can be constructed from two instances of $H_{3\text{–SAT}}$ and an auxilliary qubit, combining these leads to

$$H_{2\text{–local}}(b_1, b_2, b_3) = \lambda\Big[\sum_{i=1}^{3} H_{\text{AF}}(b_i, b_{\neg i}) + \sum_{i=1}^{8} H_{\text{AF}}(b_{a_i}, b_{\neg a_i}) + H_{\text{AF}}(b_f, b_{\neg f})$$

$$+H_{3\text{–SAT}}(b_{\neg 1}, b_{\neg 2}, b_{\neg a_1}) + H_{3\text{–SAT}}(b_{a_1}, b_{\neg 3}, b_f) + H_{3\text{–SAT}}(b_1, b_2, b_{\neg a_2}) + H_{3\text{–SAT}}(b_{a_2}, b_3, b_{\neg f})$$

$$+H_{3\text{–SAT}}(b_1, b_2, b_{\neg a_3}) + H_{3\text{–SAT}}(b_{a_3}, b_{\neg 3}, b_f) + H_{3\text{–SAT}}(b_{\neg 1}, b_{\neg 2}, b_{\neg a_4}) + H_{3\text{–SAT}}(b_{a_4}, b_3, b_{\neg f})$$

$$+H_{3\text{–SAT}}(b_1, b_{\neg 2}, b_{\neg a_5}) + H_{3\text{–SAT}}(b_{a_5}, b_3, b_f) + H_{3\text{–SAT}}(b_{\neg 1}, b_2, b_{\neg a_6}) + H_{3\text{–SAT}}(b_{a_6}, b_{\neg 3}, b_{\neg f})$$

$$+H_{3\text{–SAT}}(b_1, b_2, b_{\neg a_7}) + H_{3\text{–SAT}}(b_{a_7}, b_{\neg 3}, b_f) + H_{3\text{–SAT}}(b_{\neg 1}, b_{\neg 2}, b_{\neg a_8}) + H_{3\text{–SAT}}(b_{a_8}, b_3, b_{\neg f})\Big]$$

$$-2\, b_f + 1.$$

The terms on the first line are all to enforce the relationship between a variable and its logical inverse. Each of the next four lines assigns a value to the flag variable b_f for a state and it's logical inverse, for instance the leftmost two terms of the second line

enforce that $b_f = 0$ if $(b_1, b_2, b_3) = (0, 0, 0)$, while the right two terms enforce that $b_f = 1$ if $(b_1, b_2, b_3) = (1, 1, 1)$. Because there are $2^3 = 8$ possible bitstrings for (b_1, b_2, b_3), and each term to enforce a flag state requires two instances of $H_{3-\text{SAT}}$ (and two auxilliary bits), a total of 16 instances are required as well as 16 auxilliary bits. Finally the last line of this equation actually implements the penalty by adding an energy difference between the two states of b_f. Note that the total number of bits required to express this term is six for the logical bits and their inverses, 16 for the auxilliary qubits, and two for the flag and its inverse. The total number of bits to map this three local Hamiltonian is therefore 24.

Bibliography
- Paper showing the universality of the Ising spin models: [25].

Part II

Hamiltonians quadratic in z and linear in x (Transverse Field Ising Hamiltonians)

The Ising Hamiltonian with a transverse field in the x direction is possible to implement in hardware:

$$H = \sum_i \left(\alpha_i^{(z)} z_i + \alpha_i^{(x)} x_i \right) + \sum_{ij} \left(\alpha_{ij}^{(zz)} z_i z_j \right). \tag{53}$$

D. ZZZ-TI-CBBK: Transvese Ising from ZZZ, by Cao, Babbush, Biamonte, and Kais (2015)

There is only one reduction in the literature for reducing a Hamiltonian term to the transverse Ising Hamiltonian, and it works on 3-local zzz terms, by introducing an auxiliary qubit with label a:

$$\alpha z_i z_j z_k \to \alpha^I + \alpha_i^z z_i + \alpha_j^z z_j + \alpha_k^z z_k + \alpha_a^z z_a + \alpha_a^x x_a + \alpha_{ia}^{zz} z_i z_a + \alpha_{ja}^{zz} z_j z_a + \alpha_{ka}^{zz} z_k z_a \tag{54}$$

$\alpha^I = \frac{1}{2} \left(\Delta + \left(\frac{\alpha}{6} \right)^{2/5} \Delta^{3/5} \right)$

$\alpha_i^z = -\frac{1}{2} \left(\left(\frac{7\alpha}{6} + \left(\frac{\alpha}{6} \right)^{3/5} \Delta^{2/5} \right) - \left(\frac{\alpha \Delta^4}{6} \right)^{1/5} \right)$

$\alpha_j^z = \alpha_i^{(z)}$

$\alpha_k^z = \alpha_i^{(z)}$

$\alpha_a^z = \frac{1}{2} \left(\Delta - \left(\frac{\alpha}{6} \right)^{2/5} \Delta^{3/5} \right)$

$\alpha_a^x = \left(\frac{\alpha \Delta^4}{6} \right)^{1/5}$

$\alpha_{ia}^{zz} = -\frac{1}{2} \left(\left(\frac{7\alpha}{6} + \left(\frac{\alpha}{6} \right)^{3/5} \Delta^{2/5} \right) + \left(\frac{\alpha \Delta^4}{6} \right)^{1/5} \right)$

$\alpha_{ja}^{zz} = \alpha_{ia}^{(zz)}$

$\alpha_{ka}^{zz} = \alpha_{ja}^{(zz)}$

Including all coefficients and factorizing, we get:

$$\alpha z_i z_j z_k \to \left(\Delta + \frac{\alpha \Delta^4}{6}^{1/5} (z_i + z_j + z_k) \right) \left(\frac{1 - z_a}{2} \right) + \frac{\alpha \Delta^4}{6}^{1/5} x_a \tag{55}$$

$$+ \left(\left(\frac{\alpha}{6} \right)^{2/5} \Delta^{3/5} - \left(\frac{7\alpha}{6} + \left(\frac{\alpha}{6} \right)^{3/5} \Delta^{2/5} \right) (z_i + z_j + z_k) \right) \left(\frac{1 + z_a}{2} \right) \tag{56}$$

The low-lying spectrum (eigenvalues **and** eigenvectors) of the right side of Eq. (54) will match those of the left side to within a spectral error of ϵ as long as $\Delta = \mathcal{O}\left(\epsilon^{-5} \right)$.

Cost
- 1 auxiliary qubit

- 8 auxiliary terms not proportional to $\mathbb{1}$.

Part III

General Quantum Hamiltonians

IV.   NON-PERTURBATIVE GADGETS

A.   NP-OY (Ocko & Yoshida, 2011)

Summary
For the 8-body Hamiltonian:

$$H_{\text{8-body}} = -J \sum_{ij} \left(x_{ij3}x_{ij+1,2}x_{ij4}x_{ij+1,4}x_{i+1j1}x_{i+1j+1,1}x_{i+1j3}x_{ij+1,2} + \right.$$
$$\left. z_{ij1}z_{ij2}z_{ij3}z_{ij4} + z_{i-1j4}z_{ij1} + z_{ij2}z_{ij-1,3} + z_{ij4}z_{i+1j1} + z_{ij3}z_{ij+1,2} \right), \tag{57}$$

we define auxiliary qubits labeled by a_{ijk}, two auxiliaries for each pair ij: labeled a_{ij1} and a_{ij2}. Then the 8-body Hamiltonian has the same low-lying eigenspace as the 4-body Hamiltonian:

$$H_{\text{4-body}} = -\sum_{ij} \alpha \left(z_{ij1}z_{ij2}z_{ij3}z_{ij4} + z_{i,j,-1,4}z_{ij1} + z_{ij2}z_{i,j-1,3} + z_{ij4}z_{i+1,j,1} + z_{ij3}z_{i,j+1,2} \right.$$
$$\left(1 - z_{a_{ij1}} + z_{a_{ij2}} + z_{a_{ij1}}z_{a_{ij2}} \right) \left(z_{a_{i,j+1,1}} + z_{a_{i,j+1,2}} + z_{a_{i,j+1,1}}z_{a_{i,j+1,2}} - 1 \right) +$$
$$\left(1 + z_{a_{ij1}} - z_{a_{ij2}} + z_{a_{ij1}}z_{a_{ij2}} \right) \left(1 - z_{a_{i+1,j1}} - z_{a_{i+1,j2}} - z_{a_{i+1,j1}}z_{a_{i+1,j2}} \right) +$$
$$\frac{U}{2} \left(z_{a_{ij1}} + z_{a_{ij2}} + z_{a_{ij1}}z_{a_{ij2}} - 1 \right) +$$
$$\frac{t}{2} \left(\left(x_{a_{ij2}} + z_{a_{ij1}}x_{a_{ij2}} \right) x_{ij3}x_{ij4} + \left(x_{a_{ij1}}x_{a_{ij2}} + y_{a_{ij1}}y_{a_{ij2}} \right) x_{i,j+1,2}x_{i,j+1,4} + \right.$$
$$\left. \left(x_{a_{ij2}} - z_{a_{ij1}}x_{a_{ij2}} \right) x_{i+1,j+1,1}x_{i+1,j+1,2} + \left(x_{a_{ij1}}x_{a_{ij2}} - y_{a_{ij1}}y_{a_{ij2}} \right) x_{i+1,j,1}x_{i+1,j,3} \right) . \tag{58}$$

Now by defining the following ququits (spin-$3/2$ particles, or 4-level systems):

$$s^{zz}_{ijki'j'k'} = z_{ijk}z_{i'j'k'} \tag{59}$$
$$s^{zz}_{a_{ij}1} = \left(1 - z_{a1_{ij}} + z_{a2_{ij}} + z_{a1_{ij}}z_{a2_{ij}} \right) \tag{60}$$
$$s^{zz}_{a_{ij}2} = \left(z_{a1_{ij}} + z_{a2_{ij}} + z_{a1_{ij}}z_{a2_{ij}} - 1 \right) \tag{61}$$
$$s^{zz}_{a_{ij}3} = \left(1 + z_{a1_{ij}} - z_{a2_{ij}} + z_{a1_{ij}}z_{a2_{ij}} \right) \tag{62}$$
$$s^{xz}_{a_{ij}1} = \left(x_{a2_{ij}} + z_{a1_{ij}}x_{a2_{ij}} \right) \tag{63}$$
$$s^{xz}_{a_{ij}2} = \left(x_{a2_{ij}} - z_{a1_{ij}}x_{a2_{ij}} \right) \tag{64}$$
$$s^{xx}_{ijki'j'k'} = x_{ijk}x_{i'j'k'} \tag{65}$$
$$s^{xy}_{a_{ij}1} = \left(x_{a1_{ij}}x_{a2_{ij}} + y_{a1_{ij}}y_{a2_{ij}} \right) \tag{66}$$
$$s^{xy}_{a_{ij}2} = \left(x_{a1_{ij}}x_{a2_{ij}} - y_{a1_{ij}}y_{a2_{ij}} \right) \tag{67}$$

NP-OY (Ocko & Yoshida, 2011) [Continued]

We can write the 4-body Hamiltonian on qubits as a 2-body Hamiltonian on ququits:

$$
\begin{aligned}
H_{\text{2-body}} = -\sum_{ij} \Big(&\alpha \left(s^{zz}_{ij1ij2} s^{zz}_{ij3ij4} + s^{zz}_{ij-1,4ij1} + s^{zz}_{ij2ij-1,3} + s^{zz}_{ij4i+1j1} + s^{zz}_{ij3ij+1,2} + s^{zz}_{a_{ij}1} s^{zz}_{a_{ij+1}2} - s^{zz}_{a_{ij}3} s^{zz}_{a_{i+1j}3} \right) \\
&+ \frac{U}{2} s^{zz}_{a_{ij},1} + \frac{t}{2} \left(s^{xz}_{a_{ij}1} s^{xx}_{ij3ij4} + s^{xy}_{a_{ij}1} s^{xx}_{ij+1,2ij+1,4} + s^{xz}_{a_{ij}2} s^{xx}_{i+1,j+1,1i+1,j+1,2} + s^{xy}_{a_{ij}2} s^{xx}_{i+1j1,i+1,j3} \right) \Big).
\end{aligned}
\tag{68}
$$

The low-lying eigenspace of $H_{\text{2-body}}$ is *exactly* the same as for $H_{\text{4-local}}$.

Cost
- 2 auxiliary ququits for each pair ij.

- 6 more total terms (6 terms in the 8-body version becomes 12 terms: 11 of them 2-body and 1 of them 1-body).

Pros
- Non-perturbative. No prohibitive control precision requirement.

- Only two auxiliaries required for each pair ij.

- 8-body to 2-body transformation can be accmplished in 1 step, rather than a 1B1 gadget which would take 6 steps or an SD + $(3 \rightarrow 2)$ gadget combination which would take 4 steps.

Cons
- Increase in dimention from working with only 2-level systems (spin-1/2 particles or 2×2 matrices) to working with 4-level systems (spin-3/2 particles).

- Until now, only derived for a very specific Hamiltonian form.

- This appraoch may become more demanding for Hamiltonians that are more than 8-local.

Bibliography
- Original paper: [26].

B.   NP-SJ (Subasi & Jarzynski, 2016)

Summary
Determine the k-local term, $H_{k-\text{local}}$, whose degree we wish to reduce, and factor it into two commuting factors: $H_{k'-\text{local}}H_{(k-k')-\text{local}}$, where k' can be as low as 0. Separate all terms that are at momst $(k-1)$-local into ones that commmute with one of these factors (it does not matter which one, but without loss of generality we assume it to be the $(k-k')$-local one) and ones that anti-commute with it:

$$H^{\text{commuting}}_{<k-\text{local}} + H^{\text{anti}-\text{commuting}}_{<k-\text{local}} + \alpha H_{k'-\text{local}}H_{(k-k')-\text{local}} \tag{69}$$

Introduce one auxiliary qubit labeled by a and the Hamiltonian:

$$\alpha x_a H_{k'-\text{local}} + H^{\text{commuting}}_{<k-\text{local}} + z_a H^{\text{anti}-\text{commuting}}_{<k-\text{local}} \tag{70}$$

no longer contains $H_{k-\text{local}}$ but $H^{\text{anti}-\text{commuting}}_{<k-\text{local}}$ is now one degree higher.

Cost
- 1 auxiliary qubit to reduce k-local term to $(k'+1)$-local where k' can even be 0-local, meaning the k-local term is reduced to a 1-local one.

- Raises the k-locality of $H^{\text{anti}-\text{commuting}}_{<k-\text{local}}$ by 1 during each application. It can become $(>k)$-local!

Pros
- Non-perturbative

- Can linearize a term of arbitrary degree in one step.

- Requires very few auxiliary qubits.

Cons
- Can introduce many new non-local terms as an expense for reducing only one k-local term.

- If the portion of the Hamiltonian that does not commute with the $(k-k')$-local term has termms of degree $k-1$ (which can happen if $k'=0$) they will all become k-local, so there is no guarantee that this method reduces k-locality.

- If any terms were more than 1-local, this method will not fully quadratize the Hamiltonian (it must be combined with other methods).

- It only works when the Hamiltonian's terms of degree at most $k-1$ all either commute or anti-commmute with the k-local term to be eliminated.

Example

$$4z_5 - 3x_1 + 2z_1 y_2 x_5 + 9x_1 x_2 x_3 x_4 - x_1 y_2 z_3 x_5 \rightarrow 9x_{a_1} + 4z_{a_4} z_5 - 3z_{a_3} x_1 - z_{a_3} x_{a_4} a3 + 2x_{a_3} x_5 \tag{71}$$

Bibliography
- Original paper, and description of the choices of terms and factors used for the given example [27].

C.   NP-N (Nagaj, 2010)

Bibliography
- Original paper: [28].

V. PERTURBATIVE $(3 \to 2)$ GADGETS

The first gadgets for arbitrary Hamiltonians acting on some number of qubits, were designed to reproduce the spectrum of a 3-local Hamiltonian in the low-lying spectrum of a 2-local Hamiltonian.

A. P$(3 \to 2)$-DC (Duan, Chen, 2011)

Summary

For any group of 3-local terms that can be factored into a product of three 1-local factors, we can define three auxiliary qubits (regardless of the number of qubits we have in total) labeled by a_i and make the transformation:

$$\prod_i^3 \sum_j \alpha_{ij} s_i \to \alpha^I + \alpha_i^{ss} \sum_i \left(\sum_j \alpha_{ij} s_{ij} \right)^2 + \alpha_i^{sx} \sum_i \sum_j \alpha_{ij} s_{ij} x_{a_i} + \alpha^{zz} \sum_{ij} z_{a_i} z_{a_j} \tag{72}$$

$$\alpha^I = \frac{1}{8\Delta} \tag{73}$$

$$\alpha^{ss} = \frac{1}{6\Delta^{1/3}} \tag{74}$$

$$\alpha^{sx} = -\frac{1}{6\Delta^{2/3}} \tag{75}$$

$$\alpha^{zz} = -\frac{1}{24\Delta} \tag{76}$$

The result will be a 2-local Hamiltonian whose low-lying spectrum is equivalent to the spectrum of $H_{3-\text{local}}$ to within ϵ as long as $\Delta = \Theta\left(\epsilon^{-3}\right)$.

Cost

- 1 auxiliary qubit for each group of 3-local terms that can be factored into three 1-local factors.

- $\Delta = \Theta\left(\epsilon^{-3}\right)$

Pros
- Very few auxiliary qubits needed

Cons
- Will not work for Hamiltonians that do not factorize appropriately.

Bibliography
- Original paper: [29]

B.   P$(3 \to 2)$-DC2 (Duan, Chen, 2011)

Summary

For any 3-local term (product of Pauli matrices s_i) in the Hamiltonian, we can define *one* auxiliary qubit labeled by a and make the transformation:

$$\alpha \prod_i^3 s_i \to \alpha^I + \alpha^s s_3 + \alpha^z z_a + \alpha^{ss} \left(s_1 + s_2 \right)^2 + \alpha^{sz} s_3 z_a + +\alpha^{sx} \left(s_1 x_a + s_2 x_a \right) \tag{77}$$

$$\alpha^I = -\frac{1}{2\Delta} \tag{78}$$

$$\alpha^s = \alpha \left(\frac{1}{4\Delta^{2/3}} - 1 \right) \tag{79}$$

$$\alpha^z = \alpha \left(\frac{1}{4\Delta^{2/3}} - 1 \right) \tag{80}$$

$$\alpha^{ss} = \frac{1}{\Delta^{1/3}} \tag{81}$$

$$\alpha^{sz} = \frac{\alpha}{4\Delta^{2/3}} \tag{82}$$

$$\alpha^{sx} = \frac{1}{\Delta^{2/3}} \tag{83}$$

$$\tag{84}$$

The result will be a 2-local Hamiltonian whose low-lying spectrum is equivalent to the spectrum of $H_{3-\text{local}}$ to within ϵ as long as $\Delta = \Theta\left(\epsilon^{-3}\right)$.

Cost

- 1 auxiliary qubit for each 3-local term.

- $\Delta = \Theta\left(\epsilon^{-3}\right)$

Example

$$x_1 z_2 y_3 - 3x_1 x_2 y_4 + z_1 x_2 \to \alpha^I + \alpha^z \left(z_{a_1} + z_{a_2} \right) + \alpha^y \left(y_3 + y_4 \right) + \alpha^{zx}_{12} z_1 x_2 + \alpha^{zx} z_2 x_{a_1} + \alpha^{xx}_{11} x_1 x_2 \tag{85}$$

$$+ \alpha^{xx} \left(x_1 x_{a_1} + x_1 x_{a_2} + x_2 x_{a_2} \right) + \alpha^{yz} \left(y_3 z_{a_1} + y_4 z_{a_2} \right) \tag{86}$$

Bibliography

- Original paper: [29]

C. $P(3 \to 2)$-KKR (Kempe, Kitaev, Regev, 2004)

Summary

For any 3-local term (product of commuting matrices s_i) in the Hamiltonian, we can define three auxiliary qubits labeled by a_i and make the transformation:

$$\prod_i^3 s_i \to \alpha^I + \alpha_i^{ss} \sum_i s_i^2 + \alpha_i^{sx} \sum_i s_i x_{a_i} + \alpha^{zz} \sum_{ij} z_{a_i} z_{a_j} \tag{87}$$

$$\alpha^I = -\frac{1}{8\Delta} \tag{88}$$

$$\alpha^{ss} = -\frac{1}{6\Delta^{1/3}} \tag{89}$$

$$\alpha^{sx} = \frac{1}{6\Delta^{2/3}} \tag{90}$$

$$\alpha^{zz} = \frac{1}{24\Delta} \tag{91}$$

The result will be a 2-local Hamiltonian whose low-lying spectrum is equivalent to the spectrum of $H_{3-\text{local}}$ to within ϵ as long as $\Delta = \Theta\left(\epsilon^{-3}\right)$.

Cost

- 3 auxiliary qubits for each 3-local term.

- $\Delta = \Omega\left(\epsilon^{-3}\right)$

Example

$$x_1 z_2 y_3 - 3x_1 x_2 y_4 + z_1 x_2 \to \alpha^I + \alpha_{2a_{12}}^{zx} z_2 x_{a_{12}} + \alpha_{12}^{xx} x_1 x_2 + \alpha_{1a_{11}}^{xx} x_1 x_{a_{11}} + \alpha_{1a_{21}}^{xx} x_1 x_{a_{21}} + \alpha_{2a_{22}}^{xx} x_2 x_{a_{22}} + \alpha_{3a_{13}}^{yz} y_3 x_{a_{13}} + \alpha_{4a_{23}}^{yx} y_4 x_{a_{23}} \tag{92}$$

D. $P(3 \rightarrow 2)$-OT (Oliveira-Terhal, 2005)

Summary

For any 3-local term which is a product of 1-local matrices s_i, we can define one auxiliary qubit labeled by a and make the transformation:

$$\alpha \prod_i^3 s_i \rightarrow \alpha^I + \alpha_1^s s_1^2 + \alpha_2^s s_2^2 + \alpha_3^s s_3 + \alpha_a^z z_a + \alpha_{12}^{ss} s_1 s_2 + \alpha_{13}^{ss} s_1^2 s_3 + \alpha_{23}^{ss} s_2^2 s_3 + \alpha_{3a}^{sz} s_3 z_a + \alpha_{1a}^{sx} s_1 x_a + \alpha_{2a}^{sx} s_2 x_a \quad (93)$$

$$\alpha^I = \frac{\Delta}{2} \tag{94}$$

$$\alpha_1^s = -\frac{\alpha^{2/3} \Delta^{1/3}}{2} \tag{95}$$

$$\alpha_2^s = \frac{\alpha^{2/3} \Delta^{1/3}}{2} \tag{96}$$

$$\alpha_3^s = -\frac{\alpha^{1/3} \Delta^{2/3}}{2} \tag{97}$$

$$\alpha_a^z = -\frac{\Delta}{2} \tag{98}$$

$$\alpha_{12}^{ss} = -\Delta^{1/3} \tag{99}$$

$$\alpha_{13}^{ss} = \alpha \frac{1}{2} \tag{100}$$

$$\alpha_{23}^{ss} = \alpha \frac{1}{2} \tag{101}$$

$$\alpha_{3a}^{sz} = \frac{\alpha^{1/3} \Delta^{2/3}}{2} \tag{102}$$

$$\alpha_{1a}^{sx} = -\frac{\alpha^{1/3} \Delta^{2/3}}{\sqrt{2}} \tag{103}$$

$$\alpha_{2a}^{sx} = \frac{\alpha^{1/3} \Delta^{2/3}}{\sqrt{2}} \tag{104}$$

A k-local Hamiltonian with a 3-local term replaced by this 2-local Hamiltonian will have an equivalent low-lying spectrum to within ϵ as long as $\Delta = \Omega(\epsilon^{-3})$.

Cost

- 1 auxiliary qubit for each 3-local term.

- $\Delta = \Omega(\epsilon^{-3})$

Example

Bibliography
- Original paper where $\alpha = 1$: [30]. For arbitrary α see the 2005 v1 from arXiv, or [31]. Connection to improved version: [32].

VI.   PERTURBATIVE 1-BY-1 GADGETS

A 1B1 gadget allows k-local terms to be quadratized one step at a time, where at each step the term's order is reduced by at most one. In each step, a k-local term is reduced to $(k-1)$-local, contrary to SD (sub-division) gadgets which can reduce k-local terms to $(1/2)$-local in one step.

A.   P1B1-OT (Oliveira & Terhal, 2008)

Summary
We wish to reduce the k-local term:

$$H_{k-\text{local}} = \alpha \prod_j^k s_j. \tag{105}$$

Define one auxiliary qubit labeled by a and make the transformation:

$$H_{k-\text{local}} \rightarrow -\left(\frac{\alpha}{2}\right)^{1/3} \Delta^{2(1-r)} s_k \left(\frac{1-z_a}{2}\right) + \left(\frac{\alpha}{2}\right)^{1/3} \frac{\Delta^r}{\sqrt{2}} \left(s_{k-1} - s_{k-2}\right) x_a \tag{106}$$

$$+ \frac{1}{2}\left(\frac{\alpha}{2}\right)^{2/3} \left(\Delta^{r-1} s_{k-1} + \text{sgn}(\alpha)\sqrt{2}\Delta^{-1/4} \prod_j^{k-2} s_j\right)^2 + \frac{\alpha}{4}\left(1 + 2\text{sgn}^2\alpha\Delta^{3/2-2r}\right) s_k. \tag{107}$$

The result will be a $(k-1)$-local Hamiltonian with the same low-lying spectrum as $H_{k-\text{local}}$ to within ϵ as long as $\Delta = \Omega\left(\epsilon^{-3}\right)$.

Cost
- Only 1 auxiliary qubit.

- $\Delta = \Omega\left(\epsilon^{-3}\right)$

Example

Bibliography
- Described in: [32], based on: [30].

B. P1B1-CBBK (Cao, Babbush, Biamonte, Kais, 2015)

Summary
Define one auxiliary qubit labeled by a and make the transformation:

$$H_{k-\text{local}} \rightarrow \left(\Delta + \left(\frac{\alpha}{2} \right)^{3/2} \Delta^{1/2} s_k \right) \left(\frac{1 - z_a}{2} \right) \tag{108}$$

$$- \frac{\alpha^{2/3}}{2} \left(1 + \text{sgn}^2 \alpha \right) \left((2\alpha)^{2/3} \text{sgn}^2 \alpha + \alpha^{1/3} s_k - \sqrt[3]{2} \Delta^{1/2} \right) \left(\frac{1 + z_a}{2} \right) \tag{109}$$

$$+ \left(\frac{\alpha}{2} \right)^{1/3} \Delta^{3/4} \left(\prod_j^{k-2} s_j - \text{sgn}(\alpha) s_{k-1} \right) x_a + \text{sgn}(\alpha) \sqrt[3]{2} \alpha^{2/3} \left(\Delta^{1/2} + \Delta^{3/2} \right) \prod_j^{k-1} s_j. \tag{110}$$

The result is $(k-1)$-local and its low-lying spectrum is the same as that of $H_{k-\text{local}}$ when Δ is large enough.

Cost
- Only 1 auxiliary qubit.

- $\Delta = \Omega \left(\epsilon^{-3} \right)$

Example

Bibliography
- Described in: [32], based on: [30].

VII. PERTURBATIVE SUBDIVISION GADGETS

Instead of recursively reducing k-local to $(k-1)$-local one reduction at a time, we can reduce k-local terms to $(k/2)$-local terms directly for even k, or to $(k+1)/2$-local terms directly for odd k. Since when k is odd we can add an identity operator to the k-local term to make it even, we will assume in the following that k is even, in order to avoid having to write floor and ceiling functions.

A. PSD-OT (Oliveira & Terhal, 2008)

Summary
We factor a k-local term into a product of three factors: operators H_1, H_2 acting on non-overlapping spaces, and scalar α. Then introduce an auxiliary qubit labelled by a and make the transformation:

$$H_{k-\text{local}} \to \Delta \frac{1 - z_a}{2} + \frac{\alpha}{2} H_1^2 + \frac{\alpha}{2} H_2^2 + \sqrt{\frac{\alpha \Delta}{2}} \left(-H_1 + H_2 \right) x_a. \tag{111}$$

The resulting Hamiltonian has a degree of 1 larger than the degree of whichever factor H_1 or H_2 has a larger degree, and the low-lying spectrum is equivalent to the original one to within $\mathcal{O}(\alpha\epsilon)$ for sufficiently large Δ.

Cost
- 1 auxiliary qubit for each k-local term that can be factored into two non-overlapping subspaces, is enough to reduce the degree down to $k/2 + 1$.

- $\Delta = \frac{\alpha \left(\|H_{(\text{else})} + \Omega(\sqrt{2}) \max(\|H_1\|, \|H_2\|) \| \right)^6}{\epsilon^2} = \Omega\left(\alpha\epsilon^{-2} \right).$

Pros
- Potentially very few auxiliary qubits needed.

Cons
- Requires the ability to factor k-local terms into non-overlapping subspaces that are at most $(k-2)$-local in order to reduce k-locality. This is not possible for $z_1 x_2 x_3 + z_2 z_3 x_4$, for example.

- Δ needs to be rather large.

- Cannot reduce 3-local to 2-local unless we generalize to a factor of 3 non-overlapping subspaces instead of 2. Needs to be combined with $3- \to 2$ gadgets, for example.

- A lot of work may be needed to find the optiml reduction, since each k-local term can be factored in many ways, and some of these ways may affect the ability to reduce other k-local terms.

Example

Bibliography
- Original paper where $\alpha = 1$: [30]. For arbitrary α see the 2005 v1 from arXiv, or [31]. Connection to improved version: [32].

B.   PSD-CBBK (Cao, Babbush, Biamonte, Kais 2015)

Summary

For any k-local term, we can subdivide it into a product of two $(k/2)$-local terms:

$$H_{k-\text{local}} = \alpha H_{1,(k/2)-\text{local}} H_{2,(k/2)-\text{local}} + H_{(k-1)-\text{local}}. \tag{112}$$

Define one qubit a and make the following Hamiltonian is $(k/2)$-local:

$$\Delta \frac{1 - z_a}{2} + |\alpha| \frac{1 + z_a}{2} + \sqrt{|\alpha|\Delta/2} \left(\text{sgn}(\alpha) H_{1,(k/2-\text{local})} - H_{2,(k/2-\text{local})} \right) x_a \tag{113}$$

The result is a $(k/2)$-local Hamiltonian with the same low-lying spectrum as $H_{k-\text{local}}$ for large enough Δ. The disadvantage is that Δ has to be larger.

Cost
- $\Delta \geq \left(\frac{2|\alpha|}{\epsilon} + 1 \right) \left(|\alpha| + \epsilon + 22\|H_{(k-1)-\text{local}} \right)$

Pros
- only one qubit to reduce k to $\lceil k/2 \rceil + 1$

Cons
- Only beneficial for $k \geq 5$.

Example

Bibliography
- Original paper: [32].

VIII.   PERTURBATIVE DIRECT GADGETS

Here we do not reduce k by one order at a time (1B1 reduction) or by $k/2$ at a time (SD reduction), but we directly reduce k-local terms to 2-local terms.

A.   PD-JF (Jordan & Farhi, 2008)

Summary

Express a sum of k-local terms as a sum of products of Pauli matrices s_{ij}, and define k auxiliary qubits laelled by a_{ij} for each term i, and make the transformmation:

$$\sum_i \alpha_i \prod_j^k s_{ij} \rightarrow \frac{-k(-\epsilon)^k}{(k-1)!} \sum_i \frac{1}{2}\left(k^2 - \sum_{jl}^k z_{a_{ij}} z_{a_{il}}\right) + \epsilon\left(\alpha_i s_{i1} x_{i1} + \sum_j^k s_{ij} x_{ij}\right) - f(\epsilon)\Pi, \qquad (114)$$

for some polynomial $f(\lambda)$. The result is a 2-local Hamiltonian with the same low-lying spectrum to within ϵ^{k+1} for sufficiently smmall ϵ.

Cost
- Number of auxiliary qubits is tk for t terms.

- Unknown requirement for ϵ.

Pros
- All done in one step, so easier to implement than 1B1 and SD gadgets.

Cons
- Requires 2 more auxiliary qubits per term than 1B1-KKR.

- Unknown polynomial $f(\lambda)$

Example

Bibliography
- Original paper [33].

B.   PD-BFBD (Brell, Flammia, Bartlett, Doherty, 2011)

Summary
The 4-body Hamiltonian:

$$H_{\text{4-local}} = - \sum_{ij} \left(z_{4i+1,j} z_{4i+2,j} z_{4i+3,j} z_{4i+4,j} + x_{4i+3,j} x_{4i+4,j} x_{4i+6,j} x_{4i+4,j+1} \right) \tag{115}$$

is transformed into the 2-body Hamiltonian:

$$H_{\text{2-local}} = - \sum_{ij} \left(x_{8i+4,j} x_{8i+6,j} + x_{8i+3,j+1} x_{8i+5,j+1} + z_{8i+4,j} z_{8i+3,j+1} + z_{8i+6,j} z_{8i+5,j+1} + \right. \tag{116}$$

$$= -\lambda \left(x_{8i+1,j} x_{8i+3,j} + x_{8i+2,j} x_{8i+4,j} + x_{8i+5,j} x_{8i+6} + x_{8i+7} x_{8i+8} \right. \tag{117}$$

$$= \left. z_{8i+1,j} z_{8i+3,j} + z_{8i+2,j} z_{8i+4,j} + z_{8i+5,j} z_{8i+6} + z_{8i+7} z_{8i+8} \right)) \tag{118}$$

For $\lambda = \mathcal{O}\left(\epsilon^{-5}\right)$, the 2-local Hamiltonian has the same low-lying spectrum as the 4-local Hamiltonian, to within an error of ϵ.

Cost
- In total, uses four times the number of qubits of the original Hamiltonian.

- Unknown requirement for λ.

Pros
- All done in one step, so easier to implement than implementing two 1B1 gadgets.

- Very symmetric

Cons
- Ordinary 1B1 or SD followed by 3→2 gadgets would require half as many total qubits.

- Many 2-local terms.

- Perturbative, as opposed to NR-OY which is similar but does not involve any λ parameter.

- Required value of λ for it to work, is presently unknown.

Bibliography
- Original paper: [34].

Part IV

Appendix

IX. FURTHER EXAMPLES

Example Here we show how deductions can arise naturally from the Ramsey number problem. Consider $\mathcal{R}(4,3)$ with $N = 4$ nodes. Consider a Hamiltonian:

$$H = (1 - z_{12})(1 - z_{13})(1 - z_{23}) + \ldots + (1 - z_{23})(1 - z_{24})(1 - z_{34}) + z_{12}z_{13}z_{14}z_{23}z_{24}z_{34}. \quad (119)$$

See [5] for full details of how we arrive at this Hamiltonian.

Since we are assuming we have no 3-independent sets, we know that $(1 - z_{12})(1 - z_{13})(1 - z_{23}) = 0$, so $z_{12}z_{13}z_{23} = z_{12}z_{13} + z_{12}z_{23} + z_{13}z_{23} - z_{12} - z_{13} - z_{23} + 1$. This will be our deduction.

Using deduc-reduc we can substitute this into our 6-local term to get:

$$H = 2(1 - z_{12})(1 - z_{13})(1 - z_{23}) + \ldots + (1 - z_{23})(1 - z_{24})(1 - z_{34}) + \quad (120)$$

$$z_{14}z_{24}z_{34}(z_{12}z_{13} + z_{12}z_{23} + z_{13}z_{23} - z_{12} - z_{13} - z_{23} + 1). \quad (121)$$

We could repeat this process to remove all 5- and 4-local terms without adding any auxiliary qubits. Note in this case the error terms added by deduc-reduc already appear in our Hamiltonian.

X.   FURTHER REFERENCES

- Gadgets for pseudo-Boolean optimization problems, with reduced precision requirements: [35].

- Proof that $xx + zz$ or xz is universal: [36].

- Formalization of pseudo-Boolean gadgets in quantum language. [21].

- By adding more couplers and more auxiliary qubits, we can bring the error down arbitrarily low: [37].

- More toric code gadgets: [38].

- Parity adiabatic quantum computing (LHZ lattice): [39].

- Extensions of the LHZ scheme: [40].

- Minimizing k-local discrete functions with the help of continuous variable calculus[41].

ACKNOWLEDGMENTS

* richard.tanburn@gmail.com
† nicholas.chancellor@gmail.com
‡ nik.dattani@gmail.com

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