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Analytical framework for quantum alternating operator ansätze

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Abstract
We develop a framework for analyzing layered quantum algorithms such as quantum alternating operator ansätze (QAOA). In the context of combinatorial optimization, our framework relates quantum cost gradient operators, derived from the cost and mixing Hamiltonians, to classical cost difference functions that reflect cost function neighborhood structure. By considering QAOA circuits from the Heisenberg picture, we derive exact general expressions for expectation values as series expansions in the algorithm parameters, cost gradient operators, and cost difference functions. This enables novel interpretability and insight into QAOA behavior in various parameter regimes. For single-level QAOA\textsubscript{1}, we show the leading-order changes in the output probabilities and cost expectation value explicitly in terms of classical cost differences, for arbitrary cost functions. This demonstrates that, for sufficiently small positive parameters, probability flows from lower to higher cost states on average. By selecting signs of the parameters, we can control the direction of flow. We use these results to derive a classical random algorithm emulating QAOA\textsubscript{1} in the small-parameter regime, i.e. that produces bitstring samples with the same probabilities as QAOA\textsubscript{1} up to small error. For deeper QAOA\textsubscript{p} circuits we apply our framework to derive analogous and additional results in several settings. In particular we show QAOA always beats random guessing.

We describe how our framework incorporates cost Hamiltonian locality for specific problem classes, including causal cone approaches, and applies to QAOA performance analysis with arbitrary parameters. We illuminate our results with a number of examples including applications to QUBO problems, MaxCut, and variants of MaxSAT. We illustrate the generalization of our framework to QAOA circuits using mixing unitaries beyond the transverse-field mixer through two examples of constrained optimization problems, Max Independent Set and Graph Coloring. We conclude by outlining some of the further applications we envision for the framework.
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1. Introduction

Parameterized quantum circuits have gained much attention both as potential near-term algorithms and as new paradigms for quantum algorithm design more generally. Approaches based on quantum alternating operator ansätze (QAOA) \cite{1-5} have been extensively studied in recent years \cite{6-51}. These approaches alternate $p$ times between applications of a cost-function-based phase-separation operator and a probability-amplitude mixing operator, illustrated in figure 1. Nevertheless, relatively few rigorous performance guarantees are known in nontrivial settings, especially beyond a small constant number of circuit layers and the few specific problems studied thus far. Thus, the power and underlying mechanisms of such algorithms remains unclear, as do the problems and regimes where quantum advantage may be possible. Hence it is important to develop novel tools and approaches for analyzing and understanding such algorithms.

This analysis includes evaluating QAOA behavior and performance for both individual problem instances and for classes of problems or instances, e.g. worst- or average-case performance for instances in a class. Evaluating average behavior can be particularly useful for large $p$ since that involves many QAOA parameters. In this case, finding optimal parameters for each instance can be difficult. Instead, focusing on characteristic or average behavior can simplify parameter selection by identifying a single set of parameters that work well for typical instances of the class, as well as lead to new performance guarantees.

To help address these issues, in this paper we develop theoretical tools in the form of an analytic framework, with notation, concepts, and results, to provide better understanding of the behavior of these algorithms, their strengths and weaknesses, and ultimately to design better quantum algorithms. The main underlying ideas of our framework are as follows, and apply to computing algorithm operators and expectation values of interest:

- Quantum circuit observable expectation values can be equivalently computed by acting on the observable by the circuit (by conjugation $H \rightarrow U^\dagger H U = H + \ldots$, i.e. the Heisenberg picture), followed by taking the initial state expectation value.
- For layered circuits we can recursively conjugate to obtain exact operator series in the algorithm parameters; for alternating ansatz terms of the same or similar form will reappear in the series.
- For QAOA, in particular with the originally proposed transverse-field mixer, the resulting terms, their action, and their initial state expectation values can be related to classical functions derived from the cost function that capture its structure.

A number of useful properties for analysis are shown, including that initial state expectation values of many of the resulting terms are identically zero. For specific problem classes we can directly incorporate problem and operator locality. Further, in particular parameter regimes many such terms may be close to zero, allowing for compact approximate expressions by neglecting such terms, particularly for higher-order behavior. The expressions we derive are useful for more efficient numeric explorations of QAOA, as well as direct analytical insights. Further, the framework can be used to simplify the generation of more complicated expressions with computer algebra systems, such as for exact expressions or higher-order approximations, enabling further exploration of QAOA behavior.

Our framework can be applied to illuminate various aspects of QAOA. We illustrate the use of the framework in several general results and applications including:

- exact formulas for QAOA$_{p}$ probabilities and expectation values as power series in the algorithm angles (parameters).
- leading-order approximations for QAOA$_{p}$ expectation values and probabilities.
  * for arbitrary (nonconstant) cost functions there exist angles such that QAOA$_{p}$ beats random guessing.
  * better or more applicable approximations may be systematically obtained by including higher-order terms.
  * simple classical algorithms emulate sampling from QAOA circuits in some of these regimes, with small error.
  * identification of some general parameter regimes for which QAOA$_{p}$ performance analysis is classically tractable, particularly a regime of polynomially-small parameters, which hence precludes quantum advantage, as illustrated in figure 2.
- a generalized formalization unifying several previous approaches for deriving QAOA$_{p}$ performance bounds, encapsulating previous results for specific problems such as exact results for MaxCut; we demonstrate this approach by obtaining results for QAOA$_{1}$ on a variant of Max-2-SAT as a specific example.
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Figure 1. A Quantum Alternating Operator Ansatz circuit with \( p \) levels that alternate between application of the phase and mixing operators \( U_P \) and \( U_M \). The \( \gamma_j, \beta_j \) are parameters for these operators and \( |s\rangle \) is a suitable initial state. Our framework particularly applies to such layered quantum circuit ansätze.

Figure 2. Schematic regimes of the QAOA operator \( U_M(\beta)U_P(\gamma) \) with parameters \( \beta \) and \( \gamma \); similar ideas apply for QAOA\(_p\). The inner region indicates operators close to the identity \( I = U_M(0)U_P(0) \), corresponding to small parameters, where the QAOA probabilities and cost expectation values are characterized by the leading order terms of the exact series expressions we derive. In particular, sufficiently (i.e. inverse-polynomially) small parameters allow for efficient classical emulation generally (i.e. classical sampling up to small error). In contrast, for arbitrary parameters, efficient classical sampling from QAOA\(_1\) circuits is impossible under standard beliefs in computational complexity theory [7].

- a number of analytical and numerical examples illustrating the application of our framework to QAOA with the transverse-field mixer.
- two examples showing how our framework and results extend to quantum alternating ansätze beyond the transverse-field mixer, involving problems with different domains and encodings, or hard feasibility constraints.

Though we focus on the original QAOA, the framework naturally generalizes to other cases with structured ansätze and so would be useful for other applications, such as realizations of the variational quantum eigensolver for quantum chemistry, though in this paper we only hint at these further applications through the examples of section 5 and concluding discussion of section 6.

We remark here on some particularly related prior work. Our results build off, generalize, and unify various previous analytical approaches and results for the performance of QAOA for specific problems or in particular settings. For example, [10, 14, 17, 21, 33, 38, 39, 43, 45, 46] obtain bounds to the cost expectation value for relatively few layers. Whereas most prior work concerns specific problems or problem classes, many of our results apply to arbitrary cost functions. For MaxCut, [32, appendices 22–24] proposes a related approach for algorithmically generating polynomials capturing the QAOA cost expectation value. Another recent paper, similar in spirit to our framework though employing different technical approaches, explores a number of related but distinct viewpoints on low-depth quantum optimization [52], in particular relating the QAOA mixing operator to a graph Laplacian (of which the transverse-field mixer is a special case). Our work provides complementary insights on the connection between mixers and cost function structure. Several of recent works consider classical algorithms matching the performance of low-depth QAOA circuits [31, 43, 44]. Classical algorithms for generally computing expectation values of quantum observables are considered in [53]; in particular they show quantum circuits exponentially close to the identity can be efficiently sampled from. Our work extends this result, in the context of QAOA circuits, from exponentially small angles to polynomially small.

We emphasize that many of our formulas and results apply to QAOA circuits of arbitrary depth. As an example we consider QAOA for Grover’s unstructured search problem, and demonstrate in section 4.2 how small-angle analysis easily reproduces the result obtained rigorously in [11] that QAOA with the transverse-field mixer can reproduce the famous quadratic speedup of Grover’s algorithm.

The remainder of the Introduction gives an informal description of our framework and the results we obtained by applying it. Subsequent sections give full definitions, generalizations and precise statements of results.

1.1. Overview of analytical framework

Quantum algorithms based on QAOA utilize the noncommutativity of the cost and mixing operators in a fundamental way. From the Heisenberg perspective, a quantum circuit may be equivalently viewed as acting...
on quantum observables\(^3\) by conjugation, rather than on a quantum state (by matrix multiplication); observable expectation values may be equivalently computed as the initial state expectation of the conjugated observable. For a circuit with \(\ell\) layers, this corresponds to \(\ell\) iterated conjugation operations. In some cases this formulation gives advantages in computing or approximating expectation values. For example, this idea was applied to derive an exact formula for the level-1 QAOA cost expectation value for MaxCut in [14]. We extend these approaches to more general cost functions and settings using the correspondence between commutators and unitary conjugation (i.e. between Lie algebras and Lie groups) to derive exact expressions for relevant operators and expectation values as power series in the algorithm parameters with terms that reflect cost function structure.

For QAOA we show how the resulting operators and expectation values reflect cost function changes over neighborhoods induced by the mixing operator. For simplicity, the primary example we consider in the paper is the transverse-field mixer Hamiltonian \(B = \sum_j X_j\) and corresponding initial state \(|s\rangle := |\pm\rangle^\otimes n\) as originally proposed for the quantum approximate optimization algorithm [6], though our framework may be applied more generally. This mixer induces a neighborhood structure on classical bitstrings related to Hamming (i.e. bit-flip) distance on the Boolean cube. Different mixers induce different neighborhood structures, and our framework extends to these cases as well, as we illustrate with two examples in section 5.

At the heart of our approach is a fundamental correspondence

\[
\text{quantum operators } \longleftrightarrow \text{ classical functions}
\]

between derived operators on the space of quantum states, and classical functions that describe their behavior in terms of the structure of the cost function. The functions and operators appearing in our framework are related to discrete versions of functions and operators from vector calculus, particularly discrete difference operators. Given a mixer \(B\) and cost Hamiltonian \(C\), iteratively taking commutators generates a sequence of Hamiltonians (up to factors of \(i\)). The most fundamental such operator is their commutator

\[
\nabla C := [B, C] = BC - CB,
\]

which we call the cost gradient operator, as motivated by its action on particular quantum states. (For convenience, we will sometimes refer to higher-order commutators of \(B\) and \(C\) as cost gradients generically.) In particular, we show \(\nabla C|s\rangle = \frac{1}{\sqrt{2^n}} \sum_{x \in \{0, 1\}^n} dc(x)|x\rangle\), for the classical cost divergence function

\[
dc(x) := \sum_{j=1}^n \partial_j c(x),
\]

where \(c(x)\) is the cost function to be optimized, and \(\partial_j c(x)\) gives the change in cost for each string \(x \in \{0, 1\}^n\) with respect to flipping its \(j\)th bit (i.e. \(dc\) captures average cost function structure over single bit-flip neighborhoods). For example, \(dc(x^*) \leq 0\) is a necessary condition for \(x^*\) to maximize the cost function. We may then use properties of the functions to understand properties of the operators, and vice versa; for example we have in general \(\frac{1}{n} \sum_{x \in \{0, 1\}^n} dc(x) = \langle s|\nabla C|s\rangle = 0\).

The cost gradient \(\nabla C\) corresponds to infinitesimal conjugation of \(C\) by the QAOA mixing operator, i.e. \(e^{iB\theta}Ce^{-iB\theta} = C + i\theta \nabla C + O(\theta^2)\) as \(|\theta| \to 0\). Including additional terms leads to higher-order cost gradients (nested commutators, e.g. \(\nabla^2 C := [B, [B, C]]\), and so on) that reflect cost changes over neighborhoods of greater Hamming distance, at higher powers of the mixing angle. To include the QAOA phase operator we also require commutators with respect to \(C\), \(\nabla C := [C, \cdot]\), which act in relation to the underlying cost function \(c(x)\). Hence, treating the layers of QAOA as iterated conjugations of an observable leads to series expressions which may be used to compute or approximate expectation values and other important quantities.

As we discuss briefly in section 6, our framework can be applied to recently proposed variants of QAOA [33, 54], and more generally to layered quantum algorithms including applications beyond combinatorial optimization; in such cases the resulting operators will reflect structure resulting from both the problem and choice of ansatz.

1.2. Overview of application to QAOA

The series expansions resulting from our framework are especially informative when the leading terms in the series dominate the behavior. This is the case for the small-angle regime, i.e. when all angles in the QAOA parameter schedule are relatively small in magnitude. Hence, as a main application of our framework, we

\(^3\) Many important quantities for parameterized quantum circuits may be expressed as observable expectation values such as the expected cost and approximation ratio, or measurement probabilities.
investigate the small-angle setting for QAOA circuits generally. We analyze single-layer QAOA$_1$ in detail in section 3, and generalize to $p \geq 1$ layers (denoted QAOA$_p$ throughout) in section 4.

For QAOA$_1$, we show that, to third order in the angles $\gamma, \beta$, the probability to measure each bitstring $x$ changes from its initial value by a single contribution proportional to the cost divergence $dc(x)$ and the product $\gamma \beta$. Hence, with respect to the $2^n$-dimensional space of bitstring probabilities, to leading order QAOA is reminiscent of a step of classical gradient descent, with learning rate (step size) proportional to $\gamma \beta$. The leading-order contribution to the cost expectation then follows as the expectation of $\gamma \beta \sum_i c(x) \, dc(x)$. We emphasize the expression $\gamma \beta \sum_i c(x) \, dc(x)$ depends on both the algorithm parameter values and their ordering.

Our general results point to the tradeoff between parameter size and number of QAOA levels for potential quantum advantage. Indeed, it is known that sampling from QAOA$_p$ always beats random guessing for any nonconstant cost function.

### Table 1. Leading-order cost expectation and probabilities for QAOA$_p$ for cost function $c(x)$, which dominate in particular when the QAOA angles are small, $|\gamma|, |\beta| \ll 1$. The initial probability of measuring $x \in \{0, 1\}^n$ is $P_0(x) = \frac{1}{2^n}$ which corresponds to QAOA with all angles zero. The first two rows follow from theorem 2.2.1, and the following two rows follow from theorems 2.2.2 and 4.2.1. In each case the next contributing terms are order 4 and higher in the QAOA angles; all other terms up to order 3 are shown to be identically zero. We show the three additional terms that contribute up to fifth order explicitly in theorem 4.2.1. We emphasize the expression $\sum_{i,j} \gamma_i \beta_j$ depends on both the algorithm parameter values and their ordering.

| Quantity | Initial value | Leading-order contribution |
|----------|---------------|---------------------------|
| $P_1(x)$ | $\frac{1}{2^n}$ | $-\frac{1}{2^n} \gamma \beta \sum_i c(x)$ |
| $c^2_1$ | $\frac{1}{2^n} \sum_x c(x)$ | $-\frac{1}{2^n} \gamma \beta \sum_x c(x) dc(x)$ |
| $P_p(x)$ | $\frac{1}{2^n}$ | $-\frac{1}{2^n} \left( \sum_{i,j} \gamma_i \beta_j \right) \sum_x c(x) dc(x)$ |
| $c_p^2$ | $\frac{1}{2^n} \sum_x c(x)$ | $-\frac{1}{2^n} \left( \sum_{i,j} \gamma_i \beta_j \right) \sum_x c(x) dc(x)$ |

As a consequence, we show that the measurement outcomes of QAOA$_1$ are effectively classically emulatable in the regime of polynomially small angles. More precisely, we provide a simple classical randomized algorithm that produces bitstrings with probabilities matching the leading order behavior of QAOA$_1$, and bound the resulting error from the neglected terms for the case where $\gamma, \beta$ are bounded in magnitude by an inverse-polynomial in the problem size. (A similar argument applies to QAOA$_p$ (cf table 1), though we do not analyze the error in detail for the general $p$ case.) We use these results to show that QAOA always beats random guessing for any nonconstant cost function.

Our general results point to the tradeoff between parameter size and number of QAOA levels for potential quantum advantage. Indeed, it is known that sampling from QAOA$_p$ circuits with unrestricted parameters, even for $p = 1$, cannot be efficiently performed classically under widely believed complexity theoretic assumptions [7]. Our results take steps towards a clearer demarcation of when quantum advantage may be possible (cf figure 2). Extending the analysis to QAOA with arbitrary number of levels $p$ shows that QAOA$_p$ gives the same leading-order behavior as QAOA$_1$, with a suitable choice of effective angles for QAOA$_p$, as indicated by the quantities shown in table 1. Thus, there is no possibility of quantum advantage for QAOA$_p$ for fixed $p$ when all angles are small.

We similarly show how to obtain leading-order terms in particular cases where only some of the angles are small, which yield further generally applicable expressions. For QAOA$_1$ applied to quadratic unconstrained binary optimization (QUBO) problems, we show the case of small-mixing angle $\beta$ and unrestricted phase angle $\gamma$ can again be efficiently emulated classically, whereas this does not appear generally possible in the converse case of small phase angle but arbitrary mixing angle. The latter case can be understood in light of our framework from the fact that cost differences over neighborhoods of arbitrary Hamming distance contribute as the mixing angle grows in magnitude, which eventually become superpolynomial in size.

Application of our framework is not restricted to small angles. Including higher order terms in our series expansions results in a sequence of increasingly accurate approximations valid over larger angle regimes. Alternatively, for specific problems and relatively small $p$ we can often derive compact exact expressions using our formalism by explicitly incorporating problem structure. We give high-level algorithms computing approximate or exact QAOA cost expectation values in this way in section 4.4. Our approach yields more tractable expressions than alternative approaches to obtaining general formulas; we contrast with one such ‘sum-of-paths’ approach to QAOA in appendix A.
Table 2. Summary of important notation, with the MaxCut problem, which seeks to partition the vertices of a graph so as to maximize the number of cut edges, as an example. The top of the table shows functions on bits and the middle shows related operators on qubits. The n-qubit computational basis states $|x\rangle$ represent bitstrings $x \in \{0,1\}^n$, and the bottom of the table shows the standard QAOA initial state we primarily consider in this paper, though other choices are possible. The operators $X_i, Y_i, Z_i$ are the single qubit Pauli matrices acting on the i\textsuperscript{th} qubit. The symbols $\theta, \phi$ denote right-acting operators on functions, and likewise $D, V$ denote superoperators on the space of n-qubit matrices; in both cases k-th powers indicate operator iteration. The rightmost column shows their realization for MaxCut on a graph $G = (V, E)$ with $|V| = n$ nodes, where here the graph neighborhood of each vertex variable is denoted $N(j) = \{i : (i,j) \in E\} \subset [n]$ with $|N(j)| = \deg(j)$ the degree of vertex $j$. The formula $dc(x) = 2|E| - 4c(x)$ follows from equation (22) and is particular to MaxCut, as is the formula given for $\nabla^C C$ which is a special case of lemma 3.6.1. Similar but more complicated formulas can be derived for higher-order mixed gradients $\nabla^X X \ldots \nabla^n X \nabla^C C$ and for applications to problems other than MaxCut.

| Label                      | Symbol | Definition                                                                 | Example: value for MaxCut |
|----------------------------|--------|---------------------------------------------------------------------------|---------------------------|
| Cost function              | $c(x)$ | $c : \{0,1\}^n \to \mathbb{R}$                                          | $\sum_{i=1}^n x_i \otimes x_i$ |
| j-th partial difference    | $\delta c(x)$ | $c^{(j)}(x) - c(x)$                                                   | $|N_j| - 2 \sum_{i \in N(j)} x_i \otimes x_i$ |
| Cost divergence            | $dc(x)$ | $\sum_{i=1}^n \partial_x c(x)$                                        | $2|E| - 4c(x)$ |
| $\ell$-th cost divergence  | $d^\ell c(x)$ | $\sum_{i=1}^n \partial_x^\ell c(x)$                        | $(-4)^\ell (c(x) - |E|/2)$ |
| Mixing Hamiltonian         | $B$    | Transverse-field                                                          | $\sum_{i=1}^n X_i$ |
| Cost Hamiltonian           | $C$    | $C|x\rangle = c(x)\ket{x}$                                              | $\frac{1}{2} I - \frac{1}{2} \sum_{(i,j) \in E} Z_i Z_j$ |
| Cost divergence Hamilton. | $DC$   | $DC|x\rangle = dc(x)\ket{x}$                                           | $\frac{1}{2} \sum_{(i,j) \in E} Z_i Z_j$ |
| $\ell$-th cost div. Ham.  | $D^\ell C$ | $D^\ell C|x\rangle = d^\ell c(x)\ket{x}$                          | $\frac{1}{2} (-4)^\ell \sum_{(i,j) \in E} Z_i Z_j$ |
| Cost gradient op.          | $\nabla C$ | $[B, C]$                                                                  | $\sum_{(i,j) \in E} (Y_i Z_j + Z_i Y_j)$ |
| Order 2 cost gradient      | $\nabla^2 C$ | $[B, [B, C]]$                                                            | $\left\{ \begin{array}{ll} 4\ell^{-1} \nabla C & \text{for } \ell \text{ odd} \\ 4\ell^{-2} \nabla^2 C & \text{for } \ell \text{ even} \end{array} \right.$ |
| $\ell$-th order gradient   | $\nabla^\ell C$ | $[B, [\ldots, [B, C]]]$                                                 | (Various; see sections 2.4 and 3) |
| Gradient w.r.t. A          | $\nabla_A$ | $[A, \cdot]$                                                             | Uniform distrib. of possible cuts |
| Mixed gradient             | $\nabla_C \nabla C$ | $[C, [B, C]]$                                                             | $-\sum_{i=1}^n (|N_i| X_i + \sum_{j \in N(i)} X_i Z_j Z_j)$ |
| Initial state              | $|s\rangle$ | $|+\rangle^\otimes n = \frac{1}{\sqrt{n}} \sum_{x \in \{0,1\}^n} |x\rangle$ | $(C)_{0} = \frac{n}{2} \sum_x c(x) = |E|/2$ |

1.3. Roadmap of paper
The table of Contents gives the detailed structure of the paper. Here, we make some remarks on dependencies between the various sections.

Section 2 gives a self-contained presentation of our framework, including general cost difference functions and cost gradient operators and their properties; see table 2 below for a summary of important notation. As an immediate demonstration of our formalism we state our general leading-order results for QAOA in section 2.2, and illustrate how the framework facilitates comparison between different quantum circuit ansätze by comparing leading-order QAOA; to a quantum quench in section 2.2.1. In section 2.6, we show how to incorporate into our framework, when applicable, additional problem or instance-wise locality considerations (for example, MaxCut restricted to bounded-degree graphs), providing a basis for more refined QAOA results incorporating locality in sections 3.2 and 4.3.

Section 3 provides a detailed application of our framework to QAOA. After deriving general results, we use the framework to obtain results for QAOA for small mixing angle (but arbitrary phase) and vice versa (small phase, but arbitrary mixing angle). The section presents several examples; subsequent sections are independent of these examples.

Section 4 applies the framework to the general case of QAOA. While a number of the results in section 4 generalize those in section 3, this section can be read immediately after section 2 by those readers who wish to focus on the $p > 1$ case.

Section 5 discusses how our framework applies to QAOA using different encodings and mixers other than the transverse-field mixer. In this case, the operators in our framework are defined in terms of the neighborhood structures induced by those alternative mixers, which we illustrate with two examples of constrained problems: Maximum Independent Set and Graph Coloring. This section builds on the results of section 2, but does not directly depend on those of section 3 or section 4.

Finally, we comment on several additional applications of our framework in section 6. Some additional technical results and proofs are deferred to the Appendices and may also be read independently.

2. Analytical framework for quantum optimization
Consider a classical cost function $c(x)$ we seek to optimize over bitstrings $x \in \{0,1\}^n$, i.e. the n-dimension Boolean hypercube. For example, $c(x)$ gives the number of cut edges in MaxCut, or the number of satisfied clauses in MaxSAT. Here for clarity we assume all bitstrings encode feasible candidate solutions; we consider examples which extend our methods to optimization over non-trivial feasible subspaces in section 5.
We may encode each bitstring $x \in \{0, 1\}^n$ with the corresponding $n$-qubit computational basis state $|x\rangle$. A computational basis (Pauli $Z$) measurement of this quantum register at the end of an algorithm then returns each candidate solution $x$ with some probability $P(x)$.

Throughout the paper $n$ denotes the number of (qu)bits and $X_j, Y_j, Z_j$ denote the Pauli matrices $\sigma_x, \sigma_y, \sigma_z$ acting on the $j$th qubit, respectively.

The cost function is naturally represented as the cost Hamiltonian

$$C = \sum_x c(x)|x\rangle\langle x|$$

which acts diagonally in the computational basis as $C|x\rangle = c(x)|x\rangle$ for each $x \in \{0, 1\}^n$. In quantum algorithms such as quantum annealing or QAOA, the usual initial state is

$$|s\rangle := |+\rangle^\otimes n = \left(\frac{|0\rangle + |1\rangle}{\sqrt{2}}\right)^\otimes n = \frac{1}{\sqrt{2^n}} \sum_{x \in \{0, 1\}^n} |x\rangle$$

which gives a uniform probability distribution over bitstrings (i.e. $P_0(x) := |\langle x|s\rangle|^2 = \frac{1}{2^n}$, and $\langle c \rangle_0 = \frac{1}{n} \sum_x c(x)$), and the (transverse-field) mixing Hamiltonian

$$B := \sum_{j=1}^n X_j$$

is utilized to mediate probability flow between states.

Here we briefly review the original QAOA [3] of Farhi, Goldstone, and Gutmann, which is the main application we consider in the paper. A QAOA$_p$ circuit creates the parameterized quantum state (cf figure 1)

$$|\gamma\beta\rangle_p = U_M(\beta_p)U_P(\gamma_p)U_M(\beta_{p-1})\ldots U_P(\gamma_1)|s\rangle = e^{-i\beta_p B}\ldots e^{-i\gamma_1 C}|s\rangle$$

by applying the mixing and phase separation unitaries $U_M(\beta)$, $U_P(\gamma)$ in alternation $p$ times each to the initial state $|s\rangle = \frac{1}{\sqrt{2^n}} \sum_x |x\rangle$. The original QAOA mixing unitary $U_M(\beta) = \exp(-i\beta B)$ is specified as time evolution under the transverse-field Hamiltonian of equation (3), and the phase operator $U_P(\gamma) = \exp(-i\gamma C)$ by time evolution under the cost Hamiltonian $C$. In optimization applications typically each QAOA state preparation is followed by a measurement in the computational basis which returns some $x \in \{0, 1\}^n$ probabilistically.

For QAOA$_p$ with fixed parameters we let $P_p(x)$ denote the probability of a such a measurement returning the bitstring $x$, and $\langle C \rangle_p := \langle C \rangle_0 := \langle \gamma\beta|C|\gamma\beta \rangle$ the expected value of the cost Hamiltonian (function). More generally, we use $\langle A \rangle_p := \langle \gamma\beta|A|\gamma\beta \rangle$ to denote the QAOA$_p$ expectation value of an operator $A$. We refer generically to $\gamma_1, \beta_1, \ldots, \beta_p$ and $p$ as QAOA parameters, and will often use the term QAOA angles when the QAOA level $p$ is understood. The quantum gate depth for implementing a QAOA$_p$ circuit is related to but not the same as $p$.

Repeated preparation and measurement of a QAOA$_p$ state on a quantum computer produces a collection of candidate solution samples, with the overall best solution found returned. The samples may be used to estimate quantities such as $\langle C \rangle_p$ which in turn may be used to search for better phase and mixing angles, e.g. variationally. Alternatively, angles may be selected a priori or restricted to a specific domain or schedule.

The performance of such algorithms arise from the action of the mixing operator, which for the choice of $B$ of equation (3) relates to Hamming distances between bitstrings. Its action on quantum states can be readily interpreted in terms of classical bitstrings (with respect to the computational basis). Indeed, let $x(j)$ denote the bitstring $x \in \{0, 1\}^n$ with its $j$th bit flipped. Then from its action on basis states $X_j|x\rangle = |x^{(j)}\rangle$ we identify each Pauli operator $X_j$ as the $j$th bit-flip operator. Hence the Hamiltonian $B$ maps a given $|x\rangle$ to a superposition of strings differing from $x$ by a single bit-flip

$$B|x\rangle = \sum_{j=1}^n |x^{(j)}\rangle =: \sum_{y \in \text{nbd}(x)} |y\rangle,$$

where $\text{nbd}(x) \subset \{0, 1\}^n$ denotes the Hamming distance-1 neighbors of $x$. Thus we see that the quantum operator $B$ induces a classical neighborhood structure on the Boolean cube. Similarly, iteratively applying equation (5) one easily shows the action of $B^k$ relates to Hamming distance-$k$ neighborhoods. Indeed, for the

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4 Though different initial states or mixing Hamiltonians have been proposed to some extent in the literature, for simplicity we use $|s\rangle$ to denote the equal superposition state (equation (2)) and $B$ to denote the transverse-field Hamiltonian (equation (3)) throughout the paper. This paradigm is called X-QAOA in [41].
Example: Local cost differences

\[ \nabla c = \frac{x}{\partial c} \]

and

\[ \cos c = \arctan A \]

A related but distinct definition sometimes called the 'increases. This observation motivates a complementary sum-of-paths approach that maximizes \( e = \partial Q \) and -encodes how the cost function changes with respect to flipping the bit flips between for the 3-variable Max-2-SAT instance \( c(x) = (x_1 \lor x_2) + (x_3 \lor \bar{x}_4) \), depicted for the bottom-left corner of the Boolean cube \( x = 000 \); i.e. flipping the first or second bit increases the cost function \( \partial c(000) = \partial c(001) = 1 \), as where flipping the third decreases it \( \partial c(000) = -1 \). For problems on \( n \) variables we have \( n \) cost difference functions.

QAOA mixing operator \( U_M(\beta) = e^{-iH_B} \), the identities \( X^2 = I \) and \( [X_j, X_k] = 0 \) give \( U_M(\beta) = \prod_{j=1}^{n} (I \cos(\beta) - i \sin(\beta)X_j) \), and so its matrix elements with respect to the computational basis, \( x, y \in \{0, 1\}^n \), are

\[
(x|U_M(\beta)|y) = \cos^n(\beta)(-i \tan(\beta))^y^{(x,y)} := u_{d(x,y)},
\]

which depend only on \( \beta \) and the Hamming distance \( d = d(x,y) \) between \( x \) and \( y \).

We use this mixing neighborhood structure to build a general calculus relating classical functions encoding how the cost function changes over each neighborhood to quantum operators capturing the action of corresponding QAOA circuits. Our results formalize a number of results in prior literature concerning more specific settings. Though we focus on the transverse-field mixer (equation (3)), our results provide a guide for applying our framework to other mixers, or initial states. We consider examples of more general mixing Hamiltonians and unitaries in section 5, which naturally induce different classical neighborhoods in an analogous way. In each case the mixing operator neighborhoods are independent of the particular cost function and any neighborhood structure that it may carry.

2.1. Cost difference and cost divergence functions

The aggregate action of the QAOA phase and mixing operators fundamentally relates to the underlying (classical) operations of cost function evaluations and bit flips. To use this observation to characterize the behavior of QAOA circuits we define a sequence of classical cost difference functions derived from the cost function.

For an arbitrary cost function \( c(x) \) we define for \( j = 1, \ldots, n \) the (partial) cost difference function \( \partial c \) as

\[
\partial c(x) := c(x^{\overline{j}}) - c(x).
\]

Each \( \partial c \) encodes how the cost function changes with respect to flipping the \( j \)th bit of its input. Considering the local neighborhood of single bit flips about each bitstring \( x \) we define the cost divergence function as the total cost difference over each neighborhood

\[
dc(x) := \sum_{j=1}^{n} \delta c(x).
\]

The cost differences and divergence satisfy \( \sum_{j} \partial c(x) = \sum_{x} dc(x) = 0 \).

These functions capture information about the cost function structure. We show an example in figure 3.

For a solution \( x^* \) that maximizes \( c(x) \), we have \( \partial c(x^*) \leq 0 \) for each \( j \in [n] \), which implies \( dc(x^*) \leq 0 \). Thus \( \forall j \in [n] \partial c(x^*) \leq 0 \) gives a necessary condition for a string \( x^* \) to give a global maximum. (Likewise,

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5 The quantities \( |u_d(\beta)|, d = 1, \ldots, n \) each have a single maximum at \( \beta_d^* = \arctan \sqrt{d/(n-d)} \). This shows that state transitions of increasing Hamming weight are relatively favored as \( |\beta| \) increases. This observation motivates a complementary sum-of-paths approach discussed in appendix 4.

6 Some of our definitions to follow are labeled in analogy with familiar notions from vector calculus as an aid to identifying their behavior. However, we note important differences in our discrete domain setting.

7 A related but distinct definition sometimes called the 'jth derivative' is \( c(x|_{x_j=1}) - c(x|_{x_j=0}) \); see [35].
\[ \partial c(x^*) \geq 0 \text{ and } dc(x^*) \geq 0 \text{ for minima.} \] Hence we expect the cost divergence to be relatively large in magnitude and negative (positive) near local maxima (minima). On the other hand, for ‘typical’ bitstrings \( y \) with cost close to the mean \( \langle c \rangle_0 = \frac{1}{2^n} \sum_x c(x) \), we expect nearly as many possible bit flips will increase the cost function as decrease, which suggests \( dc(y) \simeq 0 \) for such typical strings \( y \).

2.1.1. Higher-order and mixed cost differences
We likewise consider higher-order changes in the cost function due to multiple bit flips. This follows in the usual way from considering each partial difference \( \partial_i \) as an operator mapping classical functions to classical functions \( \partial_i : c \rightarrow \partial_i c \) which may then be iterated. A useful property is the antisymmetry relation

\[ \partial_i c(x^{(\beta)}) = -\partial_i c(x). \] (9)

Applying this twice gives

\[ \partial_i^2 c(x) = \partial_i(\partial_i c(x)) = -2\partial_i c(x) \] (10)

which we write as \( \partial_i^2 c = -2\partial_i c \), and hence it follows \( \partial_i^k c = (-2)^{k-1}\partial_i c \) for \( k \in \mathbb{N} \).

For \( j \neq k \), let \( x^{(j,k)} \) denote \( x \) with its \( j \)th and \( k \)th bits flipped, and so \( |x^{(j,k)}\rangle = X_j X_k |x\rangle \). The second-order (mixed) cost difference function \( \partial_i \partial_j c \) is given by

\[ \partial_i(\partial_j c)(x) = c(x) - c(x^{(i)}) - c(x^{(k)}) + c(x^{(i,k)}) \]

which is symmetric with respect to interchange of \( j \) and \( k \). Hence, \( \partial_i \partial_j c = \partial_j \partial_i c \) so mixed difference operations mutually commute. These functions generalize to third order cost differences \( \partial_i \partial_j \partial_k c \) and higher orders in the natural way.

We may likewise iterate the cost divergence operator \( d : c \rightarrow dc \) to give

\[ d^2 c(x) := d(dc)(x) = -2dc(x) + 2\sum_{i<j} \partial_i \partial_j c(x), \] (11)

which relates to the change in cost function over the Hamming distance 2 neighborhood of each \( x \). More generally, the higher-order cost divergence \( d^k c \) is defined recursively as \( d^k c(x) := d(d(\ldots d(dc))\ldots)(x) \), which relates to the change in cost function over neighborhoods of \( k \) bit flips or less.

2.2. Application: leading-order behavior of QAOA
Before developing the operator side of our framework, we state two results relating the leading-order behavior of QAOA, generally, to the cost difference functions. The details are given in sections 3 and 4. We first consider QAOA with a single level. By expressing the action of a QAOA circuit as a series in the parameters \( \gamma, \beta \), the leading-order contributions to the measurement probabilities and cost function expectation (beyond the initial contributions \( P_0(x) = 1/2^n \) and \( \langle C \rangle_0 = \langle c \rangle_0 \) obtained from uniform random guessing) are expressible in terms of the cost divergence function. Hence, the cost divergence determines the behavior of QAOA in the ‘small-angle’ regime \( |\gamma|, |\beta| \ll 1 \); see remark 3.0.1 below, which also considers additional important quantities such as \( \| C \| \). Moreover, we show that for sufficiently small parameters QAOA behaves as an effective QAOA_1.

**Theorem 2.2.1 (Leading-order QAOA_1).** Consider QAOA_1 with an arbitrary cost function \( c(x) \). Then to lowest order in \( \gamma, \beta \) the probability \( P_1(x) \) of measuring a bitstring \( x \in \{0,1\}^n \) is given by

\[ P_1(x) \simeq P_0(x) - \frac{2\gamma \beta}{2^n} dc(x), \] (12)

with expected value of the cost Hamiltonian (cost function)

\[ \langle C \rangle_1 \simeq \langle C \rangle_0 - \frac{2\gamma \beta}{2^n} \sum_x c(x) dc(x), \] (13)

where the neglected terms in both equations are degree 4 or higher in \( \gamma, \beta \). Moreover, for any non-constant \( c(x) \) we have

\[ \sum_x c(x) dc(x) < 0. \] (14)
The theorem gives novel insight into QAOA. We see that to leading order, QAOA\textsubscript{1} causes probability to flow in (or out) of each bitstring \( x \) in proportion to its cost divergence \( dc(x) \). In particular, for a maximization problem with \( c(y) \geq 0 \) for every \( y \), when \( 0 < \gamma, \beta \ll 1 \) from equations (13) and (14) we see that to leading order probability flows to increase the cost expectation value. Similarly, selecting the product \( \gamma \beta < 0 \) guarantees that probability flows to reduce the cost expectation value, to lowest order.

As an example, for MaxCut, table 2 below has \( dc(x) = 2m - 4c(x) \), so theorem 2.2.1 gives

\[
\langle C \rangle_1 - \langle C \rangle_0 \approx -4m\gamma\beta\langle C \rangle_0 + 8\gamma\beta\langle C^2 \rangle_0 = 2\gamma\beta m
\]

to leading order for \( |\gamma|, |\beta| \ll 1 \), where notably no terms quadratic in \( m \) contribute. In particular, when \( \gamma \beta \) is positive, the change in cost function \( \langle C \rangle_1 - \langle C \rangle_0 \) is strictly positive, e.g. \( \gamma, \beta \to 0^+ \). Such information may help in initial selection and search for suitable algorithm parameters.

We bound the error arising from the neglected higher-order terms in equations (12) and (13) in section 3, from which it follows that angles can always be selected such that QAOA beats random guessing in expectation; see section 4.2.2. In terms of the solution probabilities, observe that, while not the same, the lowest order approximation equation (12) is reminiscent of a step of classical gradient descent for optimizing functions over continuous domains, in this case the 2\textsuperscript{nd}-dimensional probability vector, with ‘learning rate’ proportional to the product \( \gamma \beta \). Observe that, letting \( \tilde{P}_1(x) \) denote the righthand side of equation (12), the property \( \sum_x dc(x) = 0 \) implies \( \tilde{P}_1(x) \) gives a normalized probability distribution (assuming large enough \( n \) or sufficiently small \( |\gamma|, |\beta| \) such that \( \tilde{P}_1(x) \geq 0 \), which implies equation (12) may be interpreted classically.

Indeed, using the theorem we show a simple classical randomized algorithm based on coin flipping in section 3.1.2 that reproduces the lowest-order QAOA probabilities, and hence samples from QAOA circuits to small error in a suitably defined ‘small-angle’ regime.

The proof of theorem 2.2.1 is relatively straightforward using our framework and is given in section 3.1. We emphasize that the proof shows the other possible terms up to third order (i.e. those proportional to \( \gamma, \gamma^2, \gamma \beta, \beta^2, \beta^3, \gamma^2 \beta \) or \( \gamma \beta^2 \)) to be identically zero in both equations (12) and (13), in general. We show the nonzero contributing terms up to fifth order explicitly in section 4. Furthermore, we show that for any cost Hamiltonian given as a linear combination of Pauli Z operators \( C = a_0 I + \sum_j a_j Z_j + \sum_{i<j} a_{ij} Z_i Z_j + \ldots \), the quantity \( \frac{1}{m} \sum_x c(x) dc(x) \) appearing in equation (13) may be efficiently computed from the Hamiltonian coefficients \( a_{ij} \); see lemma 2.5.3 below.

For \( p > 1 \) layers we similarly derive leading order expansions for QAOA\textsubscript{p}, with respect to all or some angles being treated as expansion parameters, in section 4.2. As remarked, the leading order contribution to probabilities and cost expectation for QAOA\textsubscript{p} is shown to be of the same form as that of QAOA\textsubscript{1}, but with a generalized coefficient that depends on all \( 2p \) phase and mixing angles.

**Theorem 2.2.2 (3rd order QAOA\textsubscript{p}).** For QAOA\textsubscript{p}, we have cost expectation

\[
\langle C \rangle_p = \langle C \rangle_0 - \frac{2}{2^p} \sum_{1 \leq i < j \leq p} \gamma_i \beta_j \sum_x c(x) dc(x) + \ldots
\]

where the terms not shown to the right are order four or higher in \( \gamma_1, \beta_1, \ldots, \gamma_p, \beta_p \).

**Remark 2.2.1.** Theorems 2.2.1 and 2.2.2 apply more generally than stated. Viewed as expansions about the Identity operator \( I \), i.e. the QAOA circuit with all parameters set to 0, we immediately obtain corresponding results about any choice of parameters \( \gamma_j', \beta_j' \) such that the resulting QAOA circuit becomes equal or proportional to \( I \). In such cases the resulting expansions are given in terms of the parameter differences \( \gamma_j - \gamma_j' \) and \( \beta_j - \beta_j' \).

Indeed, QAOA circuits are often periodic: equation (6) shows that the QAOA mixing operator \( U_m(\beta) \) is proportional to the Identity when \( \beta \) is an integer multiple of \( \pi \), and hence \( \langle C \rangle_p \) is (at least) \( \pi \)-periodic in each mixing angle \( \beta_j \). The periodicity of the phase operator \( U_p(\gamma) \) relates to the coefficients of the cost Hamiltonian, which are uniform for many problems (e.g. MaxCut) and hence lead to similar insights (cf equation (74)). For simplicity we do not deal explicitly with periodicity of QAOA circuits in the remainder of the paper, though similar considerations apply to many of our results to follow.

### 2.2.1. Example: leading-order QAOA versus a simple quench

Our framework facilitates comparison between different quantum circuit ansätze, in particular by allowing a term-by-term comparison of the resulting series expressions. To illustrate this we show that to leading order the QAOA cost expectation value is the same as that of a simple quantum quench algorithm, where for a fixed Hamiltonian \( H = aC + bB \) the state \( |\tau\rangle := e^{-i\tau H}|s\rangle \) is prepared and measured in the computational basis. Such a quantum approach to classical optimization is considered, e.g. in [56, 57].
Proposition 2.2.1. Let $\tau > 0$, $\gamma, \beta \in \mathbb{R}$, and Hamiltonian $H$ be such that $\tau H = \sqrt{2} \beta B + \sqrt{2} \gamma C$. Then a quench of $H$ for time $\tau$ produces the same leading-order change (equation (13)) in $\langle C \rangle$ as QAOA$_1(\gamma, \beta)$, i.e.

$$\langle C \rangle_\tau = \langle \tau | C | \tau \rangle = \langle C \rangle_0 - \frac{2\gamma\beta}{2^n} \sum_x c(x) dc(x) \ldots \quad (16)$$

where the terms to the right are order four or higher in $\gamma, \beta$.

For QAOA$_p$, similarly, selecting instead $\gamma, \beta \in \mathbb{R}$ such that $\gamma \beta = \sum_{i \leq j} \gamma_i \beta_j$ gives $\langle C \rangle_\tau$ as in equation (15).

Hence, QAOA with sufficiently small parameters resembles a short-time quench. As we show, our framework allows for simple derivation of such formulas. Higher order contribution terms may be systematically derived within our framework.

Remark 2.2.2. A simple quench conserves $H$ in expectation $\langle H \rangle_\tau = \langle H \rangle_0$, so for $H = aC + bB$ linearity gives $a(\langle C \rangle_\tau - \langle C \rangle_0) = -b(\langle B \rangle_\tau - \langle B \rangle_0) = bn - b\langle B \rangle_\tau$, and thus the change in $\langle C \rangle$ is determined from the change in $\langle B \rangle$. As $-n \leq \langle B \rangle \leq n$ for any quantum state $|\tau\rangle$, we have $|\langle C \rangle_\tau - \langle C \rangle_0| \leq 2|b/a|n$ for any possible quench time $\tau$. Therefore, when $b/a$ is constant, the above quench can shift the expectation value of $C$ by at most $O(n)$, whereas $|\langle C(x^*) \rangle_\tau - \langle C \rangle_0|$ may in general be much larger (e.g. $O(n^2)$ for MaxCut). This shows the limitations of a simple quench, i.e. the quench time or ratio $|b/a|$ must often grow with the problem size if large improvements in the expected value of the cost function are sought. Alternatively, to circumvent this requirement, the Hamiltonian $B$ can be replaced or augmented with additional $k$-local terms as proposed in [56]. QAOA does not in general obey a similarly simple conservation law.

In the remainder of section 2 we derive the operators used in our framework and show the connection to the cost difference functions, as well as a number of useful properties. For the convenience of the reader we both summarize our main notation in table 2 and as an guiding example show its explicit realization for MaxCut, an NP-hard constraint satisfaction problem considered extensively for QAOA [3, 14, 15, 17, 19, 24].

2.3. Hamiltonians representing cost differences

For a cost function $c : \{0, 1\}^n \rightarrow \mathbb{R}$ with corresponding $n$-qubit diagonal Hamiltonian $C$ given in equation (1), i.e. acting as $C|x\rangle = c(x)|x\rangle$ for each $x \in \{0, 1\}^n$, we may uniquely express $C$ as a multinomial in the Pauli $Z$ operator basis as

$$C = a_0 I + \sum_{j=1}^{n} a_j Z_j + \sum_{i \leq j} a_{ij} Z_i Z_j + \ldots \quad (17)$$

We say $C$ is $k$-local for $k$ the largest degree of a nonzero term in equation (17); we further discuss problem and Hamiltonian locality considerations in section 2.6. The coefficients $a_{ij}$ of $C$ are given by the Fourier expansion of the cost function $c(x)$; see [58] for details. In particular the Identity coefficient $a_0 = \frac{1}{2^n} \sum_x c(x)$ is the cost expectation under the uniform probability distribution.

For example, for constraint satisfaction problems with cost function given by a sum of clauses $c = \sum_j c_j$, with each clause acting on at most $k$ variables, $k = O(1)$, we may efficiently construct a $k$-local cost Hamiltonian of the form equation (17) with a number of terms polynomial in $n$. For such cost Hamiltonians the corresponding QAOA phase operator $U_P(\gamma) = e^{-\gamma C}$ is efficiently implementable in terms of single-qubit and CNOT gates [58]. Motivating examples are the NP-hard optimization problems MaxCut and Max-2-SAT, studied for QAOA in [3, 8, 14, 59], which each have quadratic cost Hamiltonians.

Using the results of [58] we may similarly lift the classical partial difference and cost divergence functions of equations (7) and (8) to diagonal Hamiltonians $\partial_j C$ and $DC = \sum_j \partial_j C$, respectively, which act on computational basis states $|x\rangle$ as $\partial_j C|x\rangle = \partial_j c(x)|x\rangle$ and $DC|x\rangle = dc(x)|x\rangle$. In particular, given a cost Hamiltonian $C$ explicitly as in equation (17), the operators $\partial_j C$ and $DC$ are easily computed from the useful relations

$$\partial_j C = X_j CX_j - C, \quad (18)$$

$j = 1, \ldots, n$, from which it trivially follows that

$$\langle s | \partial_j C | s \rangle = 0 \quad \text{and} \quad \langle s | DC | s \rangle = 0. \quad (19)$$

Results such as equations (18) and (19) apply generally to any cost Hamiltonian.

---

8 Throughout the paper diagonal operators are with respect to the computational basis.
Next observe that from the Pauli anti-commutation relation \( \{X, Z\} := XZ + ZX = 0 \), the action of \( X_j \cdot X_j \) on \( C \) either flips the sign of or leaves alone each term of \( C \) in equation (17). Hence if for each \( j \) we define a partition of the terms of \( C \) as \( C = C^{(1)} + C^{(\ell)} \), where \( C^{(1)} \) is defined as the partial sum of the terms of equation (17) that contain a \( Z_j \) factor, and \( C^{(\ell)} \) the remainder, then

\[
\partial_j C = -2C^{(1)}. \tag{20}
\]

For example, for MaxCut, \( C^{(1)} \) contains a \( ZZ \) term for each neighbor (adjacent vertex) of the \( j \)th vertex. Summing over \( j \), the cost divergence Hamiltonian satisfies

\[
DC = -2 \sum_{j=1}^n C^{(1)}. \tag{21}
\]

Each strictly \( k \)-local term in \( C \) appears \( k \) times in the sum above. We may alternatively partition a \( k \)-local Hamiltonian as \( C = C_{(0)} + C_{(1)} + \cdots + C_{(k)} \), where each \( C_{(j)} \) contains strictly \( j \)-local terms. Then we also have

\[
DC = -2(C_{(1)} + 2C_{(2)} + \cdots + kC_{(k)}). \tag{22}
\]

Thus we see that for general cost Hamiltonians \( C \), we may represent \( DC \) either in terms of the problem locality (i.e. the problem graph structure reflected in the \( C^{(1)} \)) as in equation (21), or operator locality of \( C \) as in equation (22). Both of these representations of \( DC \) are useful in our analysis to follow.

Furthermore, it is often useful to view \( D : C \to DC \) as a superoperator on the space of diagonal Hamiltonians. Iterating this operation \( D^\ell C := D(D(\ldots (DC)\ldots) \ldots) \) gives

\[
D^\ell C = (-2)^\ell \sum_{j=0}^{\ell} \binom{\ell}{j} C^{(j)} \tag{23}
\]

for \( \ell = 0, 1, 2, \ldots, \) so we see \( D^\ell C \) closely relates to \( C \) (and moreover \( d^\ell \epsilon \) relates to \( \epsilon \) similarly). Hence if \( C \) is strictly \( k \)-local, then \( D^\ell C = (-2k)^\ell C \) is proportional to \( C \), and so they represent the same classical function up to a constant [58]. For example, the cost Hamiltonian for MaxCut is \( 2 \)-local, up to its Identity term; see table 2.

**Remark 2.3.1.** An important family of diagonal Hamiltonians are the projectors

\[
H_y := |y\rangle\langle y| \quad \text{for} \quad y \in \{0, 1\}^n, \tag{24}
\]

which as observables give the probability of measuring the string \( x \) for a generic state \( |\psi\rangle \) in expectation as

\[
P_x(\psi) = |\langle y| \psi \rangle|^2 = \langle \psi | H_y | \psi \rangle. \]

Importantly, \( H_y \) represents the classical function \( \delta_y(x) \) in the sense of equation (1) which is 1 when its input \( x \) equals \( y \) and 0 otherwise.

### 2.4. Cost gradient operators

Non-diagonal operators generated by (iterated) commutators of \( B \) and \( C \) play a fundamental role in our approach to analyzing QAoA. Specifically, given a cost Hamiltonian \( C \), we identify the commutator of \( B \) and \( C \) as the **cost gradient operator** \( \nabla C := [B, C]_j \), with \( \nabla := [B, \cdot] \). We refer to \( \nabla C \) as a ‘gradient’ from its action on computational basis states \( |x\rangle \), and on the equal superposition state \( |s\rangle = \frac{1}{\sqrt{n}} \sum_x |x\rangle \), which is easily expressed in terms of the cost difference functions is reminiscent of vector calculus over the reals [10].

Observe that \( \nabla C \) is skew-adjoint and traceless; in general we can make \( \nabla C \) into a Hamiltonian if we multiply by \( \pm i \).

First consider the commutators \( \nabla_j C := [X_j, C] = X_j C - CX_j, j = 1, \ldots, n \), so that \( \nabla C = \sum_{j=1}^n \nabla_j C \). For each computational basis state \( |x\rangle \) we have

\[
\nabla_j C |x\rangle = (c(x) - c(x^{(j)})) |x^{(j)}\rangle = -\partial_j c(x) |x^{(j)}\rangle.
\]

9 Commutator operators such as \( \nabla = [B, \cdot] \) are often called *adjoint operators* and written \( ad_B := \nabla \), sometimes with an additional \( i = \sqrt{-1} \) factor \( ad_B := i\nabla \) in the context of Lie algebras [60]. These operators are *inner derivations* on matrices, i.e. they satisfy the Leibniz property \( \nabla (C_1 C_2) = \nabla (C_1) C_2 + C_1 \nabla (C_2) \); see e.g. [61, section 5].

10 Our notion of gradient is distinct from others in the literature, e.g. the (vector calculus) gradient of the classical function \( f(\hat{\theta}) := \langle \psi | U(f(\hat{\theta}) A U(\hat{\theta}) | \psi \rangle \) for a parameterized quantum circuit \( U(\hat{\theta}) | \psi \rangle \) [62].
Comparing the action on basis states, we may relate the operators \( \partial_j C \) and \( \nabla_j C \) as \( \nabla_j C = \partial_j C x_j = -X_j \partial_j C \). Thus we have

\[
\nabla C(x) = -\sum_{j=1}^{n} \partial_j c(x) |x^{(j)}\rangle,
\]

and it follows

\[
\nabla C(s) = \frac{1}{\sqrt{2^n}} \sum_{x} dc(x)|x\rangle.
\]

Hence \( \langle x|\nabla C|x\rangle = 0 \) for each \( x \in \{0,1\}^n \), and \( \langle s|\nabla C|s\rangle = 0 \) from \( \sum_x dc(x) = 0 \).

The superoperator \( \nabla := [B, \cdot] \) mapping \( C \) to \( \nabla C \) cannot increase the locality of each Pauli term in \( C \) of equation (17), as \( B \) is a sum of 1-local terms, and hence the resulting number of terms in the Pauli expansion of \( \nabla C \) can increase at most by a multiplicative factor of \( k \) for \( k \)-local \( C \). For problems with cost Hamiltonians of bounded locality, e.g. QUBO problems, we can easily calculate \( \partial_j C \) and \( \nabla C \) explicitly, as demonstrated in table 2.

### 2.4.1. Higher-order gradients

To connect our framework to QAOA circuits, consider the QAOA mixing operator \( U_M(\beta) = e^{-i\beta B} \). The superoperator \( i\nabla \) is the infinitesimal generator of conjugation by \( U_M \), i.e.

\[
e^{i\beta B} C e^{-i\beta B} = C + \sum_{k=1}^{\infty} \frac{(i\beta)^k}{k!} \nabla^k C =: e^{i\beta \nabla} C.
\]

We will elaborate on and use this relationship extensively in section 3. From this perspective our formalism naturally generalizes to include higher-order gradients

\[
\nabla^\ell C := [B, [B, [B, \ldots, [B, [B, C]]]]\ldots]].
\]

\( \nabla^\ell C \) is skew-adjoint for \( \ell \) odd and self-adjoint (i.e. a Hamiltonian) for \( \ell \) even.

Our notation evokes but differs from that of vector calculus. The symbol \( \nabla^2 \) denotes ‘\( \nabla \cdot \nabla \)’ in the latter, i.e. denotes the Laplacian operator, whereas in our notation \( \nabla^2 := \nabla \nabla \) and \( \nabla C := [B, [B, C]] \). Indeed, we may instead identify \( \nabla^2 C \) with the Hessian of \( c(x) \) from its action on basis states

\[
\nabla^2 C(x) = -\sum_{j=1}^{n} \partial_j c(x) |x\rangle + \sum_{j<k} \partial_j \partial_k c(x) |x^{(j,k)}\rangle.
\]

Hence for each computational basis state \( x \) we have \( \langle x|\nabla^2 C|x\rangle = -2dc(x) \). On the uniform superposition state, the symmetry \( \partial_j \partial_k c(x^{(j,k)}) = \partial_k \partial_j c(x) \) gives

\[
\nabla^2 C(s) = \frac{1}{\sqrt{2^n}} \sum_x d^2 c(x)|x\rangle,
\]

where \( d^2 c(x) \) is defined in equation (11). This implies \( \langle s|\nabla^2 C|s\rangle = \frac{1}{n} \sum_x d^2 c(x) \).

More generally, for an operator \( A \) which acts on \( |s\rangle \) as \( A|s\rangle = \frac{1}{\sqrt{2^n}} \sum_x a(x)|x\rangle \) for a real function \( a(x) \), it follows

\[
\nabla A |s\rangle = \frac{1}{\sqrt{2^n}} \sum_x da(x)|x\rangle.
\]

This equation is useful for computing the action and expectation values of higher-order cost gradients, as we shall see in section 2.5. In particular this relates the action of \( \nabla^\ell C \) on \( |s\rangle \) to higher order cost divergence functions \( d^\ell c(x) \) as

\[
\nabla^\ell C|s\rangle = \frac{1}{\sqrt{2^n}} \sum_x d^\ell c(x)|x\rangle.
\]

In lemma 2.5.2 below we show \( \langle \nabla^\ell C \rangle_0 := \langle s|\nabla^\ell C|s\rangle = 0 \) for \( \ell \in \mathbb{Z}_+ \) and any cost Hamiltonian, which implies \( \sum_x d^\ell c(x) = 0 \) for any cost function. Note \( \langle \nabla^\ell C \rangle_{\psi} \neq 0 \) in general.
Remark 2.4.1. From the discussion for $\nabla C$ above, if $C$ is $k$-local then so is $\nabla^\ell C$, and the number of Pauli terms in $\nabla^\ell C$ is at most $k^\ell \cdot \binom{\ell}{j} = O(k^n \ell^k)$. Hence, when $k = O(1)$, if $\ell = O(\log n)$ the number of terms remains $\text{poly}(n)$ and so we can represent and compute $\nabla^\ell C$ efficiently as a linear combination of Pauli terms. For arbitrary cost Hamiltonians with $\text{poly}(n)$ Pauli terms, the same argument applies for $\ell = O(1)$.

2.4.2. Directional and mixed gradients
To extend equation (27) to include the QAOA phase operator, we require still more general notions of gradient operators. Directional cost gradients are defined as commutators of the cost Hamiltonian taken with respect to a general $n$-qubit operator $A$ as

$$\nabla A C := [A, C], \quad (33)$$
corresponding to the superoperator $\nabla_A := [A, \cdot]$. Our above definition satisfies $\nabla := \nabla_B$. Trivially, two compatible linear operators $A, G$ commute if and only if $\nabla_A G = \nabla_G A = 0$. Further observe $\nabla_A$ is linear in $A$ as $\nabla_{cA} = c \nabla_A$ for $c \in \mathbb{C}$ and $\nabla_{A + G} = \nabla_A + \nabla_G$.

Gradients with respect to the cost Hamiltonian $\nabla_C := [C, \cdot]$ naturally arise in analysis of QAOA. Generally, higher-order (mixed) gradients of $C$ will likewise reflect the structure of the cost function over neighborhoods of increasing Hamming distance. Clearly, $\nabla_C C = 0$ and $\nabla_C B = -\nabla C$. The operator $\nabla_C \nabla C := [C, [B, C]]$ is easily shown to act on basis states as

$$\nabla_C \nabla C |x\rangle = -\sum_{j=1}^n (\partial_j c(x))^2 |x(j)\rangle, \quad (34)$$

and on the initial state $|s\rangle$ as

$$\nabla_C \nabla C |s\rangle = \frac{1}{\sqrt{2^n}} \sum_x \left( -\sum_{j=1}^n (\partial_j c(x))^2 \right) |x\rangle = \frac{1}{\sqrt{2^n}} \sum_x \left( c(x) dc(x) - \sum_{j=1}^n c(x^{(j)}) \partial_j c(x) \right) |x\rangle,$$

which implies $\langle \nabla_C \nabla C |s\rangle = \frac{1}{2^n} \sum_x c(x) dc(x) \leq 0$ for all cost Hamiltonians $C$; see lemma 2.5.3 below. Similarly, for $\ell = 1, 2, 3, \ldots$, it follows from induction that

$$\nabla_C^\ell \nabla C |x\rangle = -\sum_{j=1}^n (\partial_j c(x))^{\ell+1} |x(j)\rangle, \quad (35)$$

which using $\partial_j c(x^{(j)}) = -\partial_j c(x)$ gives

$$\nabla_C^\ell \nabla C |s\rangle = \frac{-1}{\sqrt{2^n}} \sum_{j=1}^n (-\partial_j c(x))^{\ell+1} |x\rangle. \quad (36)$$

Finally, from the Jacobi identity [60] for Lie algebras it follows that any triple of $n$-qubit operators $F, G, A$ satisfy

$$\nabla_F \nabla_G A + \nabla_A \nabla_F G + \nabla_G \nabla_A F = 0. \quad (37)$$

Applying this property to $B, C$, and $\nabla C$ gives the useful identities

$$\nabla \nabla C \nabla C = \nabla \nabla^2 C, \quad (38)$$

which in particular implies $\nabla \nabla \nabla \nabla C = \nabla^3 \nabla^2 C$. Similarly, in general we have

$$\nabla \nabla C A = -\nabla_A \nabla C = (\nabla \nabla C - \nabla C \nabla) A \quad (39)$$

for any matrix $A$ acting on $n$-qubits\footnote{Equation (39) implies that ‘gradients with respect to gradients’ can be written in terms of gradients with respect to $B$ and $C$, for example we have $\nabla \nabla \nabla C = \nabla \nabla \nabla C - \nabla \nabla \nabla C$, $\nabla \nabla \nabla C = -\nabla \nabla \nabla C$ and $\nabla \nabla \nabla C = -\nabla \nabla \nabla C$.}. Further such identities may be derived, e.g. by applying higher-order Jacobi identities [63], or when considering particular problems.
2.4.3. General gradient operators

General higher-order mixed cost gradient operators \( \nabla_{A_{1}} \cdots \nabla_{A_{n}} \) follow in the natural way. We refer to \( \sum b_{i} \) as the order of a gradient operator, where for convenience we refer to all such operators as cost gradient operators. We remark that nested commutators similarly appear in a number of quantum computing applications such as, e.g., analysis of Hamiltonian simulation with Trotter-Suzuki formulas [64].

We give the following general characterization of general gradients with respect to \( B \) and \( C \) that will appear in our application to QAOA.

**Lemma 2.4.1.** For \( C, C' \) diagonal Hamiltonians (representing classical cost functions as in equation (1)), we define the general cost gradient operator

\[
A = \nabla^{b_{1}} \nabla^{b_{2}} \cdots \nabla^{b_{l}} \nabla^{b_{l+1}} C.
\]  

(40)

for \( (b_{1}, b_{2}, \ldots, b_{l}) \) a tuple of positive integers. Then \( A \) has the following properties:

(a) \( A \) is a real matrix with respect to the computational basis: \( a_{xy} := \langle x | A | y \rangle \in \mathbb{R} \).

Hence, there exists a real function \( a(x) \) such that \( A | s \rangle = \frac{1}{\sqrt{2^{n}}} \sum_{y} a(x) | y \rangle \).

(b) \( A \) is traceless, which implies \( \sum_{x} a_{xx} = 0 \), and \( A \) is either self- or skew-adjoint:

1. If \( \sum b_{i} \) is even then \( A^\dagger = A \), which implies \( a_{xy} = a_{yx} \) for each \( x, y \in \{0, 1\}^{n} \).
2. Else if \( \sum b_{i} \) is odd then \( A^\dagger = -A \), which implies \( a_{xx} = 0 \) (i.e. \( A \) has no diagonal part), and \( a_{xy} = -a_{yx} \) for each \( x, y \in \{0, 1\}^{n} \).

(c) Each tuple \( (b_{1}, b_{2}, \ldots, b_{l}) \subset \{1, 2, 3, \ldots\}^l \) identifies a cost gradient operator (equation (40)). However this labeling is not canonical as it is many-to-one.

Here we have considered distinct \( C, C' \) for generality, as we often but not always have \( C' = C \) in application of the lemma.

**Proof.** The first point follows from expanding each of the commutators in \( A \) in turn to give a linear combination of ordered products of \( B, C, \) and \( A \). As each matrix multiplication consists of strictly real quantities, the resulting computational basis matrix elements \( a_{xy} \) of \( A \) are real and \( A \) acts on \( | s \rangle \) as \( A | s \rangle = \frac{1}{\sqrt{2^{n}}} \sum_{y} \langle \sum_{x} a_{xy} | y \rangle | x \rangle \).

The second point follows from the definition of the commutator, and the cyclic property and linearity of the trace operation. Points b.1 and b.2 follow observing the commutator of a self-adjoint and a self- (skew-)adjoint operator is skew- (self-)adjoint, and applying the first point. For the third point, equation (38) shows the mapping from positive integers is not injective in general.

Each \( A = \nabla^{b_{1}} \nabla^{b_{2}} \cdots \nabla^{b_{l}} C \) may be uniquely decomposed into its diagonal and off-diagonal parts \( A = A_{\text{diag}} + A_{\text{non-diag}} \) with respect to the computational basis, such that \( \langle A \rangle_{0} = \langle A_{\text{non-diag}} \rangle_{0} \) and \( \nabla C A = \nabla C A_{\text{non-diag}} \). In the skew-adjoint case \( A_{\text{diag}} = 0 \). In the self-adjoint case, we have corresponding real functions \( a(x) = a_{\text{diag}}(x) + a_{\text{non-diag}}(x) \), with \( \sum_{x} a_{\text{diag}}(x) = 0 \). We will use these properties in the proofs of appendix B.

2.5. Initial state expectation values

We next show several results concerning the computation of initial state expectation values of cost gradient operators, which show their dependence on the cost difference functions; roughly speaking, powers of \( \nabla C \) correspond to powers of the cost function \( c(x) \) and its coefficients, whereas powers of \( \nabla \) correspond to cost differences over greater Hamming distances. Looking forward to our application to QAOA, we will derive relevant expectation values as series expressions in the algorithm parameters and initial state expectation values of different cost gradients; these lemmas allow us identify a significant fraction of the resulting terms to be identically zero which greatly simplifies our results and proofs. Some additional results are given in appendix B.

Observe that the expectation value of any \( n \)-qubit matrix \( A \) with respect to \( |s\rangle = \frac{1}{\sqrt{2^{n}}} \sum_{x} |x\rangle \) relates to the trace of \( A \) as

\[
\langle A \rangle_{0} = \frac{1}{2^{n}} \text{tr}(A) + \frac{1}{2^{n}} \sum_{y \neq x} \langle y | A | x \rangle,
\]  

(41)

where we recall our notation \( \langle A \rangle_{0} := \langle s | A | s \rangle \). When \( A \) is diagonal \( A = a_{0} I + \sum_{j} a_{j} Z_{j} + \sum_{i<j} a_{ij} Z_{i} Z_{j} + \ldots \) this becomes \( \langle A \rangle_{0} = \frac{1}{2^{n}} \text{tr}(A) = a_{0} \). Hence, lemma 2.4.1 implies a necessary condition for the initial state.
expectation value of a gradient operator (equation (40)) to be nonzero is that its order (sum of the exponents \( \sum b_j \)) is even.

**Lemma 2.5.1.** Let \( C' \) be diagonal. If \( \sum b_j \) is odd then \( \langle \nabla^{b_1} \nabla^{b_2} \ldots \nabla^{b_L} C' \rangle_0 = 0 \).

**Proof.** Follows from case b.2 of lemma 2.4.1 using that the parity of \( \sum b_j \) determines the adjointness of \( \nabla^{b_1} \nabla^{b_2} \ldots \nabla^{b_L} C' \), and applying equation (41). \( \square \)

We next show two results concerning more specific cases.

**Lemma 2.5.2.** For any \( n \)-qubit linear operator \( A \) and \( \ell \in \mathbb{Z}_+ \) we have \( \langle \nabla^\ell A \rangle_0 = 0 \).

**Proof.** For \( \ell = 1 \) as \( B|s\rangle = n|s\rangle \) we have \( \langle s|BA|s\rangle = \langle s|BA|s\rangle = (n - n) \langle s|A|s\rangle = 0 \). The general result follows inductively considering \( \nabla^\ell A = B(\nabla^\ell - 1 A) - (\nabla^\ell - 1 A)B \).

In particular, the lemma implies \( \langle \nabla^\ell C \rangle_0 = 0 \) for any cost Hamiltonian \( C \) and \( \ell \in \mathbb{Z}_+ \).

**Remark 2.5.1.** The results of lemmas 2.4.1, 2.5.1, and 2.5.2 extend to more general QAOA initial states and mixing Hamiltonians in a straightforward way. In particular, the result and proof of lemma 2.5.2 only requires that the initial state is some eigenvector of the mixing Hamiltonian. Similar considerations apply to a number of our results to follow.

**Lemma 2.5.3.** For a cost Hamiltonian \( C = a_0 I + \sum_{i<j} a_{ij} Z_i Z_j + \ldots \) we have

\[
\langle \nabla C \rangle_0 = \frac{2}{2^n} \sum_x c(x) dc(x) = -\frac{1}{2^n} \sum_j \sum_i (\partial_i c(x))^2
\]

\[
= -4 \left( \sum_j a_{j}^2 + \sum_{i<j} 2a_{ij}^2 + \sum_{i<j<k} 3a_{ijk}^2 + \ldots \right)
\]

which implies \( \langle \nabla C \rangle_0 \leq 0 \). Moreover, \( \langle \nabla^2 C \rangle_0 = \langle \nabla^2 C \rangle_0 = \langle \nabla^3 C \rangle_0 = 0 \).

**Proof.** For \( \langle \nabla C \rangle_0 \), the first two equalities follow from equations (34) and (35) which imply \( \nabla C = -\sum (\partial_i C) X_i \), and hence \( \langle \nabla C \rangle_0 \leq 0 \) always. The third equality follows expanding as a Pauli sum \( \nabla C = -4 \sum_{\sigma} a_{\sigma} \sum_i \sigma_i X_i + \ldots \) where \( \sigma \) denotes tuples of strictly increasing qubit indices as in the definition of \( C \), and any Pauli terms not shown to the right each contain at least one \( Z \) factor and so from equation (41) have 0 expectation with respect to \( |s\rangle \). The final statement follows directly from lemma 2.5.1. \( \square \)

Results for higher-order gradients may be similarly derived. In appendix B we show the next (order 4) nonzero cost gradient expectations to be

\[
\langle \nabla C \rangle_0 = \frac{2}{2^n} \sum_x c(x) dc(x),
\]

\[
\langle \nabla^2 C \rangle_0 = \frac{1}{2^n} \sum_x \sum_{j=1}^n (\partial_j c(x))^4,
\]

\[
\langle \nabla^3 C \rangle_0 = \langle \nabla C \rangle_0 \langle \nabla C \rangle_0 = \frac{2}{2^n} \sum_x \sum_{j<k} (\partial_j c(x))^2 \partial_j c(x).
\]

The first equality of equation (45) follows from equation (37). Generalizing equations (43) and (44) to \( \ell = 1, 3, 5 \ldots \) gives \( \langle \nabla^\ell C \rangle_0 = \frac{2}{2^n} \sum_x c(x) d^\ell c(x) \) and \( \langle \nabla^\ell C \rangle_0 = \frac{1}{2^n} \sum_x \sum_{j=1}^n (\partial_j c(x))^4 \), respectively, or 0 for \( \ell \) even. Such quantities may be efficiently computed from the Pauli basis coefficients of the cost Hamiltonian \( C \); cf lemma 2.5.3. We show such expressions for QUBO problems in lemma B.0.2 of appendix B. In general these expressions reveal dependence on the cost function structure. For example, an important term for analyzing QAOA for MaxCut is \( \langle \nabla^2 C \rangle_0 \), which depends on the number of triangles in the problem graph and is zero in triangle-free cases; cf section 3.6.
2.6. Problem and Hamiltonian locality considerations

For the sake of generality and notational clarity, so far we have considered arbitrary cost functions \(c(x)\). For specific problems the cost function typically has additional structure we may directly incorporate into our framework when computing various quantities of interest such as expectation values. Here we elaborate on the generalization of our framework to incorporate locality, which we further consider in the context of QAOA in section 3.2 and QAOA\(_p\) in section 4.3; see in particular table 3.

Recalling the discussion of section 2.3, consider an objective function \(c(x) = \sum_{j=1}^{m} c_j(x)\), with corresponding cost Hamiltonian \(C = \sum_{j=1}^{m} C_j\).\(^{12}\) Assume each \(c_j\) acts on a subset \(N_j \subset [n]\) of the variables \(x_1, \ldots, x_n\) (i.e. flipping variable values in \([n] \setminus N_j\) does not change \(c_j(x)\)). Then each \(C_j\) acts nontrivially only on the qubits indexed by \(N_j\) and so is \([N_j]\)-local. For example, \(|N_j| = 2\) for MaxCut, and \(|N_j| = k\) for Max-\(k\)-SAT where each \(c_j\) is a \(k\)-variable Boolean clause. We identify \(N_j\) similarly for non-diagonal Pauli terms and Hamiltonians.

To explicitly take advantage of Hamiltonian locality we will sometimes use \(|S\rangle\) to denote an operator restricted (in the obvious way) to a subset \(S \subset [n]\) of the qubits or variables.\(^{13}\) For example, 
\[
d|_{\{1,2\}} c := \partial_1 c + \partial_2 c \text{ and } \nabla |_{\{1,2\}} C := |X_1, C + |X_2, C|.
\]
Hence, for each \(c_j\) and corresponding \(C_j\), the cost divergence of \(c_j\) reduces to a sum over \(n_j\) bit flips
\[
dc_j(x) = d|_{N_j} c_j(x) = \sum_{i \in N_j} \partial_i c_j(x),
\]
and similarly
\[
DC_j = D|_{N_j} C_j = \sum_{i \in N_j} \partial_i C_j.
\]
When each \(C_j\) consists of a single Pauli \(Z\) term equations (21) and (22) imply \(DC_j = -2|N_j| C_j\).

Hence, considering the product structure of \(|s\rangle = |+\rangle^{\otimes n}\), quantities of interest may often be evaluated by considering only a relevant subset of qubits or variables. In particular, the operator \(\nabla C_j = \nabla|_{N_j} C_j\) acts on \(|s\rangle\) as (cf equation (26))
\[
\nabla C_j|s\rangle = \frac{1}{\sqrt{2^n}} \sum_x dc_j(x)|x\rangle = \left(\frac{1}{\sqrt{2^{|N_j|}}} \sum_{x \in \{0,1\}^{|N_j|}} dc_j(x)|x\rangle\right) \otimes |+\rangle^{\otimes |N| - |N_j|}
\]
(46)
where \(C_j|x\rangle = c_j(x)\), and \(\{0,1\}^{|N_j|}\) denotes bitstrings over the variables in \(N_j\). The term in parenthesis is guaranteed to be efficiently computable classically when \(|N_j|\) is a constant or scales as \(O(\log n)\). Hence it is relatively straightforward to incorporate locality where applicable into our framework. In particular, for any operator \(A\) and \(S \subset [n]\) we have \(\langle A|s\rangle = \langle +\rangle^{\otimes S} A|s\rangle = \langle +\rangle^{\otimes S} \langle +\rangle^{\otimes |S|} \langle +\rangle^{\otimes |S|} = \frac{1}{2^m} \langle +\rangle^{\otimes S} A|s\rangle = \langle +\rangle^{\otimes S} A|s\rangle^{\otimes S}\). For example, \(\langle \nabla^\ell C_j|0\rangle = 0\) for \(\ell \in \mathbb{N}\) from lemma 2.5.2, and adapting the proof of lemma 2.5.3 gives
\[
\langle \nabla c \nabla C_j|0\rangle = \frac{2}{2^n} \sum_x c(x) dc_j(x) = \frac{2}{2^n} \sum_{x \in \{0,1\}^n} c(x) dc_j(x),
\]
(47)
which becomes \(\langle \nabla c \nabla C_j|0\rangle = -4d^2\) when \(C_j\) is a single Pauli term \(C_j = a_i Z_i \ldots Z_{i_n}\). By linearity this gives \(\langle \nabla c \nabla C_j = \sum_j \langle \nabla c \nabla C_j\rangle|0\rangle\). Similar considerations will apply to higher order cost gradients as we further discuss in sections 3.2 and 4.3.

3. Applications to QAOA\(_1\)

As employed, for instance, in the QAOA performance analysis of [14, 17] for specific problems, it is often advantageous to consider QAOA circuits from the Heisenberg perspective i.e. as acting by conjugation on an observable \(C\) rather than acting on a state directly. The Heisenberg picture naturally has a number of applications in quantum computing, e.g. [65]. Indeed, for a QAOA\(_p\) circuit \(Q = U_M(\beta_p) \ldots U_1(\gamma_1)\) we have

\(^{12}\) Clearly such decompositions are not unique. The two most useful for our purposes are when each \(C_j\) corresponds to a problem clause \(c_j\), or when each \(C_j\) corresponds to a single Pauli \(Z\) term in \(C\). For the latter case it is sometimes convenient to include factors or the identity in \(C_j\) which does not affect gradients (commutators) of \(C_j\) nor QAOA dynamics.

\(^{13}\) More precisely, for an operator expressed as a sum of Pauli terms \(A = \sum_{\alpha} c_{\alpha} \sigma_\alpha\) and \(S \subset [n]\), we define \(A_{|S}\) to be the operator obtained by discarding any terms that act on qubits outside of \(S\).
so computing the QAOA\_p expectation value of the cost function, for any \( p \), is equivalent to computing the initial state expectation value of the time evolved (conjugated) observable \( U^p C U \). Here, we consider application of our framework from this perspective to QAOA\_1. In section 4 we generalize our result to QAOA\_p.

First consider a general \( n \)-qubit Hamiltonian \( H \) and corresponding unitary \( U = e^{-itH} \) for \( t \in \mathbb{R} \). From the perspective of Lie groups and algebras [60, 66], the superoperator \( i\mathbf{H}_t = i[tH, \cdot] \) is the infinitesimal generator of conjugation by \( U \), i.e. \( e^{it\mathbf{H}_t} = U^t \cdot U \). Explicitly, acting on an operator \( A \) we have

\[
U^t AU = A + it\nabla H A + \frac{(it)^2}{2} \nabla^2 H A + \frac{(it)^3}{3!} \nabla^3 H A + \ldots.
\]  

Thus we can express conjugation by an operator \( U = e^{-itH} \) in terms of gradients \( \nabla H \). Such superoperator expansions are also familiar from quantum information theory, e.g. the Liouvillian representation of unitary quantum channels [67]. Iterating this formula, the QAOA\_1 operator \( Q = Q(\gamma, \beta) = U_M(\beta)U_p(\gamma) \) acts by conjugation as to map the cost Hamiltonian \( C \rightarrow Q^1 CQ \) to a linear combination of cost gradient operators. We show several exact series expansions for QAOA\_1 with arbitrary cost function (Hamiltonian).

**Lemma 3.0.1.** Let \( A \) be an \( n \)-qubit matrix. The QAOA operator \( Q = U_M(\beta)U_p(\gamma) \) acts by conjugation on \( A \) as

\[
Q^1 AQ = \sum_{\ell=0}^{\infty} \sum_{k=0}^{\ell} \frac{(i\gamma)^\ell(i\beta)^k}{\ell!k!} \nabla^\ell C \nabla^k A.
\]  

**Proof.** Identifying \( Q^1 AQ \) as conjugation of \( A \) by \( U_M(\beta) \), followed by conjugation by \( U_p(\gamma) \), the result then follows from two applications of equation (48).

Observe we may write equation (49) succinctly as

\[
Q^1 AQ = e^{i\gamma \nabla C} e^{i\beta \nabla} A,
\]  

where the order-of-operations of the superoperators \( e^{i\gamma \nabla C} \) and \( e^{i\beta \nabla} \) is implicitly understood. Hence all terms in \( Q^1 CQ \) are of the form \( \nabla^\ell C \nabla^k C \), i.e. containing at most one alternation of \( \nabla \) and \( \nabla C \). In section 4 we apply this formula recursively to obtain analogous formulas for QAOA\_p consisting of terms containing at most \( 2p - 1 \) such alternations.

**Remark 3.0.1.** Equations (49) and (50) are invariant under the rescalings \( (\gamma, C) \rightarrow (\gamma/a, aC) \) or \( (\beta, B) \rightarrow (\beta/b, bB) \) for any \( a, b > 0 \). Hence to apply these formulas perturbatively one must consider the quantities \( \|C\| = \gamma \|C\| \) and \( \|B\| = \beta \|B\| \) as small parameters, not just \( |\gamma|, |\beta| \). We consider such a small-angle regime in section 3.1. Note that rescaling \( C \) without proportionately rescaling \( c(x) \) preserves the solution structure but would violate the condition equation (1); we assume \( c(x) \) uniquely determines \( C \) as in equation (1) throughout.

We apply lemma 3.0.1 to derive exact expressions for the cost expectation and probabilities of QAOA\_1 using \( \langle C_1 \rangle = \langle Q^1 CQ \rangle_0 \) and \( P_1(x) = \langle Q^1 H_x Q \rangle_0 \) for \( H_x := |x\rangle \langle x| \) from remark 2.3.1.

**Theorem 3.0.1.** Let \( C \) be a cost Hamiltonian. For QAOA\_1, the cost expectation is

\[
\langle C_1 \rangle = \langle C \rangle_0 - \gamma \beta \langle \nabla C \nabla C \rangle_0 + \sum_{\ell+k\geq4, \ell+k\text{even}} \frac{(i\gamma)^\ell(i\beta)^k}{\ell!k!} \langle \nabla^\ell C \nabla^k C \rangle_0,
\]

where \( \langle \nabla C \nabla C \rangle_0 = \frac{1}{2^n} \sum_x c(x) dc(x) \leq 0 \), and the probability of measuring \( x \in \{0, 1\}^n \) is

\[
P_1(x) = P_0(x) + \sum_{\ell+k\text{even}} \frac{(i\gamma)^\ell(i\beta)^k}{\ell!k!} \langle \nabla^\ell C \nabla^k H_x \rangle_0,
\]

where \( H_x := |x\rangle \langle x| \), and both sums are over subsets of integers \( \ell, k > 0 \).

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14 The Baker–Campbell–Hausdorff formula [60] allows one to similarly express the effective Hamiltonian \( H = H(\gamma, \beta) \) of each QAOA layer \( Q = U_M(\beta)U_p(\gamma) = \exp(-iH) \) as a series in commutators of \( B \) and \( C \),

\[
H = \beta B + \gamma C - \frac{\gamma^2}{2} \nabla C - \frac{\beta^2}{2} \nabla^2 C + \frac{\gamma^2 \beta}{12} \nabla^2 C \nabla^2 C + \frac{\gamma^3 \beta}{24} \nabla^3 C \nabla^2 C + \ldots,
\]

but with more complicated expressions for higher-order terms as compared to equation (49).
Proof. Plugging $A = C$ into equation (49), using $[C, C] = 0$, and taking expectation values with respect to $|s\rangle$ gives the QAOA$_1$ cost expectation value

$$
\langle C \rangle_1 = \langle s | C Q C | s \rangle = \langle C \rangle_0 + \sum_{\ell=0}^{\infty} \sum_{k=0}^{\infty} \frac{(i\tau)^\ell (i\beta)^k}{\ell! k!} \langle \nabla_C^\ell \nabla^k C \rangle_0.
$$

(51)

From lemmas 2.5.2 and 2.5.3, the lowest order nonzero contribution $\langle C \rangle$ is the second-order term $-\gamma \beta \langle \nabla_C \nabla C \rangle_0 = \frac{\gamma}{2} \beta \sum_x c(x) d_c(x)$, and the remaining terms with $\ell + k$ odd are identically zero from lemma 2.5.1, which gives the first result.

The probability result follows similarly. Applying equation (49) to $H_p := |y\rangle \langle y|$ gives

$$
P_1(y) = \langle Q^\dagger H_p Q \rangle_0 = \sum_{\ell=0}^{\infty} \sum_{k=0}^{\infty} \frac{(i\tau)^\ell (i\beta)^k}{\ell! k!} \langle \nabla_C^\ell \nabla^k H_p \rangle_0,
$$

(52)

to which using $[C, H_p] = 0$ and again applying lemma 2.5.1 gives the stated result.

We generalize this result to QAOA$_p$ in theorem 4.2.1 in section 4. We now use the leading order terms of theorem 3.0.1 to characterize QAOA$_1$ in small-parameter regimes.

3.1. Leading-order QAOA

This section provides the proofs of the results stated in section 2.2.

Proof of theorem 2.2.1. The results follow applying lemma 2.5.3 to the leading order terms of theorem 3.0.1, as $\langle \nabla_C \nabla C \rangle_0 = \frac{\gamma}{2} \sum_x c(x) d_c(x) \leq 0$ and $\langle \nabla_C \nabla H_x \rangle_0 = \frac{\gamma}{2} \sum_y c(y) d_\delta(y) = \frac{\gamma}{2} d_c(x)$ for $H_x = |x\rangle \langle x|$ of remark 2.3.1. When $c(x)$ is nonconstant then its Hamiltonian representation $C = a_0 + \sum_i a_i Z_i + \sum_i c_i a_i Z_i + \cdots$ has at least one nonzero Pauli coefficient $a_i$, $\alpha \neq 0$, and so lemma 2.5.3 implies $\langle \nabla_C \nabla C \rangle_0 < 0$.

The proof of theorem 2.2.2 is similar and given in section 4.2.1. Comparing to our results of theorems 2.2.1, 2.2.2, and 3.0.1 we see that by selecting $\tau H = \sqrt{\tau} B + \sqrt{\tau} C$ for a simple quantum quench, the lowest-order contribution to $\langle C \rangle$ is the same as for QAOA.

Proof of proposition 2.2.1. Observe that $\tau \nabla_H = \nabla_{\tau H}$ and hence $\tau \nabla_H C = \sqrt{\tau} \nabla C$ and $\tau^2 \nabla_H^2 C = 2\gamma \beta \nabla C + 2\beta^2 \nabla^2 C$. Applying equation (48) to conjugation of $C$ by $e^{-i H \tau}$ gives

$$
e^{i H \tau} C e^{-i H \tau} = C + i \tau \nabla_H C - \frac{\tau^2}{2} \nabla_H^2 C + \cdots
$$

(53)

Taking initial state expectation values of both sides and applying lemma 2.5.3 gives equation (16). The statement for QAOA$_p$ follows similarly.

3.1.1. Small-angle error bound

Here we derive rigorous error bounds to the leading-order approximations of theorem 2.2.1.

Here, the spectral norm $\| C \| := \| C \|_2$ is the maximal eigenvalue in absolute value. For a maximization problem with $c(x) \geq 0$, e.g. a constraint satisfaction problem, the norm gives the optimal cost $\| C \| = \max_x c(x)$. Here we write $C = a_0 I + C_2$ as in equation (17), with $C_2$ traceless.

Corollary 3.1.1. Let $\tilde{P}_1(x)$, $\langle C \rangle_1$ denote the probability and cost expectation estimates (equations (12) and (13)) of theorem 2.2.1 for QAOA$_1$ with a $k$-local cost Hamiltonian $C = a_0 I + C_2$, and let $0 < \varepsilon < 1$.

- If $|\gamma| \leq \frac{\varepsilon}{2 \min (\| C_2 \|, \| C \|)}$ and $|\beta| \leq \frac{\varepsilon}{2 \sqrt{\tau}}$ then

$$
\left| \langle C \rangle_1 - \langle C \rangle_1 \right| < \min (\| C_2 \|, \| C \|) \varepsilon.
$$

(54)

- If additionally or instead $|\beta| < \frac{1}{2} \frac{\varepsilon}{\sqrt{\tau}}$ then for each $x \in \{0,1\}^n$ we have

$$
\left| P_1(x) - \tilde{P}_1(x) \right| < \frac{\varepsilon}{2 \tau}.
$$

(55)
The proof is shown in appendix C through a sequence of general lemmas. For example, for MaxCut we have $\|C_Z\| = m/2 \leq \max_x c(x) = \|C\|$. Typically $\|C_Z\| < \|C\|$, but this is not true for arbitrary $C$, which is the reason for the minimum function of equation (54). Furthermore, the difference in the ranges for $\beta$ between the two cases of corollary 3.1.1 arises because measurement probabilities $P_i(x)$ correspond to $n$-local observables.

As for optimization applications we typically are interested in the expected approximation ratio $(C_I/\epsilon_{opt} \geq (C)/\|C\|$ (for maximization) achieved by a QAOA circuit, here we have selected the ranges of $\gamma, \beta$ for equation (54) such that the resulting error bound contains a factor $\|C\|$ (or $\|C_Z\|$). Hence $O(\|C\|\epsilon)$ error estimate for the expected approximation ratio. A general bound for the error of the cost expectation estimate of theorem 2.2.1 as a polynomial in $\gamma, \beta$ is given in lemma C.2.2, which may be used to alternatively select the ranges of $\gamma, \beta$ and resulting error bound. The proof of lemma C.2.2 is shown using a recursive formula that may be extended to obtain similar bounds when including higher-order terms beyond the approximations of theorem 2.2.1, as indicated in theorem 3.0.1.

3.1.2. Small-angle QAOA behaves classically

The above results imply that QAOA can be classically emulated in the small-angle regime, in the following sense: we show a simple classical randomized algorithm for emulating QAOA1 with sufficiently small $|\gamma|, |\beta|$ that reproduces the leading-order probabilities $P_i(x)$ of sampling each bitstring $x$ from theorem 2.2.1. For $|\gamma|, |\beta|$ polynomially small in the problem parameters such that the conditions of corollary 3.1.1 are satisfied this implies the same error bounds equations (54) and (55) apply for the classical algorithm.

Specifically, assume the cost function $c(x)$ can be efficiently evaluated classically. Let $K$ be a bound such that $|\beta_x(c)| \leq K$ for all $j, x$; for example, for MaxCut, we may set $K = 2$ times the maximum vertex degree in the graph. For an arbitrary cost Hamiltonian we may always take $K = 2\|C\|$ (or, $K = 2\|C_Z\|$ for $C = a_0I + C_Z$). Consider the following simple classical randomized algorithm.

**Algorithm 1.** Sample according to leading-order QAOA1.

1. Input: parameters $\gamma, \beta \in [-1, 1]$ such that $|\gamma\beta| \leq \frac{1}{2\pi}$.
2. Select a bitstring $x_0 \in \{0, 1\}^n$ and an index $j \in [n]$ each uniformly at random.
3. Compute $\partial_j(c(x_0))$ and let $\delta(x_0, j) := 2n\gamma\beta \partial_j(c(x_0))$.
4. Using a weighted coin, flip the $j$th bit of $x_0$ with probability given by $\frac{1}{2} + \frac{1}{2} \delta(x_0, j)$.
5. Return the resulting bitstring $x_1$.

By the choice of algorithm parameters in Step 1 we have $-1 \leq \delta(x, j) \leq 1$ which ensures the probability distribution resulting from Step 4 remains normalized. For sufficiently small $\gamma, \beta$ this algorithm emulates QAOA1 up to small error.

**Theorem 3.1.1.** Consider a cost Hamiltonian $C = a_0I + C_Z$. For fixed $0 < \epsilon < 1$, let $|\beta| \leq \frac{\epsilon}{2\sqrt{2K}}$ and $|\gamma| \leq \epsilon^{1/4} / (2 \min(\|C_Z\|, \|C\|))$. Then there exists an efficient classical randomized algorithm producing bitstring $x$ with probability $P_{\text{class}}(x)$ which satisfies

$$|P_{\text{class}}(x) - P_1(x)| \leq \frac{\epsilon}{2^n}.$$  \hspace{1cm} (56)

and expected value of the cost function $|\langle \hat{c}_{\text{class}} \rangle - \langle C \rangle_1| < \|C_Z\|\epsilon$.

In this sense we say that QAOA1 behaves classically in the small-angle regime.

**Proof.** Consider the conditions of the theorem imply $|\gamma\beta| \leq 1/(9n \min(\|C_Z\|, \|C\|))$ and hence $\gamma, \beta$ satisfy the first condition of algorithm 1. The probability of this procedure returning a particular bitstring $x$ is

$$\Pr(x_1 = x) = \Pr(x_0 = x) \sum_j \Pr(j) \Pr(\text{coin} = 0) + \sum_j \Pr(x_0 = x^{(j)}) \Pr(j) \Pr(\text{coin} = 1)$$

$$= \frac{1}{2^n} \sum_j \frac{1}{2} - \frac{1}{2} \delta(x, j) + \sum_j \frac{1}{2^n} \frac{1}{2} \delta(x^{(j)}, j)$$

$$= \frac{1}{2^n} \left( \sum_j \frac{1}{2} + \frac{1}{2} \sum_j \delta(x, j) \right) + \frac{1}{2^n} \left( \sum_j \delta(x^{(j)}, j) \right)$$

$$= \frac{1}{2^n} \sum_j \delta(x, j)$$

$$= \Pr(x_0 = x) - \frac{2}{2^n} \gamma\beta dc(x)$$
where we have used \( \delta(x^i, j) = -\delta(x, j) \). Observe that from \( \sum x dc(x) = 0 \) the resulting distribution remains normalized. Hence the expected value of the cost function \( c(x) \) is

\[
\langle c \rangle = \sum x \Pr(x_i = x)c(x) = \langle c(x) \rangle_0 - 2\gamma\beta(x)dc(x)_0.
\]

and so we see Algorithm 1 reproduces the leading-order probability and cost expectation estimates of theorem 2.2.1. The error bounds then follow directly from corollary 3.1.1.

Theorem 3.1.1 demonstrates that QAOA parameters must necessarily be not-too-small for potential quantum advantage. In practice, the parameter search space may be pruned in advance to avoid such regions.

3.2. Causal cones and locality considerations for QAOA1

Here we consider problem and Hamiltonian locality for QAOA1 circuits, building off of section 2.6. We extend these results to QAOA2 in section 4.3. Our framework formalizes here similar observations made in the original QAOA paper [6] in the context of computing the cost expectation \( \langle C \rangle_p \) and resulting bound to the approximation ratio, as well as subsequent work computing such quantities analytically or numerically for specific problems [14, 17], and approaches to computing or approximating quantum circuit observable expectation values more generally [53, 68].

In particular we show how using locality in our framework allows for a more direct method of dealing with the action of the QAOA phase operator. This is especially advantageous in cases where each variable appears in relatively few clauses (e.g. MaxCut on bounded degree graphs, as considered for QAOA in [3, 14]). Such cases allow for straightforward evaluation in our framework by providing succinct efficiently computable expressions of relevant quantities such as \( \langle \gamma | \nabla C | \gamma \rangle \) and \( \langle \gamma | \nabla^2 C | \gamma \rangle \) which appear for instance in both the leading-order and exact analysis of QAOA1 of sections 3.3 and 3.6.

Consider a cost Hamiltonian \( C = a_0 I + \sum_{j=1}^m C_j \) such that each \( C_j \) is a single Pauli term. As observed in [3], in cases where the problem locality is such that for the resulting cost Hamiltonian: i) each \( C_j \) acts on at most \( k \) qubits and ii) each qubit appears in at most \( D \) terms, this information can be taken advantage of in computing each \( C_j \), especially when \( k, D \ll n \), by a priori discarding operators that can be shown to not contribute\(^\text{15}\). This reduced number of necessary qubits and operators for computing expectation values is often called the (reverse) causal cone or lightcone in the literature [42, 53, 68–70], and relates to Lieb–Robinson bounds concerning the speed of propagation of information [71]. See in particular [64, section IV.B] for applications to simulating local observables. We use the nomenclature QAOA2-­cones, which we define below and in Table 3.

Recall from Section 2.3 we may decompose \( C \) with respect to \( C(i) \) the (sum of) terms in \( C \) containing a \( Z_i \) factor, \( i = 1, \ldots, n \), from which equation (20) satisfy \( \partial_C = -2C(i) \) (i.e. each \( C(i) \) is diagonal and represents the function \( -\frac{1}{2}\partial_x(c(x)) \)). Consider the operator \( \tilde{B} := U_0^bBU_p \), which will appear in our analysis to follow. Using \( B = \sum_{i=1}^n X_i \) and \( XZ = -ZX \) we have

\[
\tilde{B} = U_0^bBU_p = \sum_{i=1}^n e^{2\gamma i}C(X_i) = \sum_{i=1}^n e^{-i\partial_x C}X_i = \sum_{i=1}^n X_i e^{i\partial_x C},
\]

which implies \( \tilde{B}|s\rangle = \sum_{j=1}^n e^{-i\partial_x C}|s\rangle = \sum_{j=1}^n \sum_{i=1}^n e^{-i\partial_x C}|x\rangle \). As each Hamiltonian \( \partial_C \) only acts on qubits adjacent to \( i \) with respect to \( C = \sum_{j=1}^m C_j \), equation (57) reflects the QAOA1-­cone structure of the

\(^\text{15}\) On the other hand, while causal cone considerations are useful for computing quantities such as \( \langle C \rangle = \sum C_j \) in the case, e.g. of bounded-degree CSPs, for evaluating QAOA probabilities they may be less useful as \( H_k = |x\rangle \langle x| \) is \( n \)-local. This observation motivates the general result of theorem 3.0.1.
particular problem. Hence for each \( C_j, j = 1, \ldots, m \), acting on qubits \( N_j \subset [n] \), define the superset
\[
L_j = N_j \cup \{ \ell : \exists j' \neq j \text{ s.t. } \ell \in N_j \cap N_{j'} \},
\]
(58)
which we refer to as the QAOA-\( 1 \)-cone of \( C_j \). In section 4.3 we generalize this to \( L_{j, \beta} \) for QAOA\( \beta \) with \( L_{j,1} = L_j \) and \( L_{j, \beta} := N_j \) as summarized in table 3.

Turning to cost gradient operators, equation (57) implies the phase operator acts on \( \nabla C \) as
\[
e^{i\gamma C} \nabla C e^{-i\gamma C} = [\hat{B}, C] = \nabla \hat{B} C = \sum_{j} \nabla P_{\ell}^{i} C_{j}.
\]
(59)
In particular terms in \( C \) that do not act entirely within \( L_j \) always commute through and cancel in each \( e^{i\gamma C} \nabla C_{j} e^{-i\gamma C} \). Hence using \( X|s\rangle = |s\rangle \) with equations (46) and (57) gives
\[
\langle \gamma | \nabla C|\gamma \rangle = i \langle \gamma | \sum_{j \in \ell} (e^{i\gamma C} - e^{-i\gamma C}) C_{j}|\gamma \rangle = -\frac{2}{2^n} \sum_{x} c(x) \sum_{i=1}^{n} \sin(\gamma \partial_{i} c(x))
\]
(60)
where for each \( C_{j} = a_{j}Z_{j_{1}} \ldots Z_{j_{|j|}} \) from equation (59) we have
\[
\langle \gamma | \nabla C_{j}|\gamma \rangle = -\frac{2}{2^{|j|}} \sum_{x \in \{0,1\}^{j}} c_{j}(x) \sum_{i \in j} \sin(\gamma \partial_{i} c_{j}(x)),
\]
(61)
and so reduces to a sum over at most \(|L_j|\) variables, with \( \langle \gamma | \nabla C|\gamma \rangle = \sum_{j} \langle \gamma | \nabla C_{j}|\gamma \rangle \).

Observe that \(|L_{j}|\) gives an upper bound to the necessary number of variables to sum over, i.e. we can compute equation (61) by summing over \( 2^{|L_{j}|} \) bitstrings. Alternatively as \(|L_{j}|\) becomes large we may approximate quantities such as equations (60) and (61) with, for example, Monte Carlo estimates.

For \( \nabla^{2} C \), a similar calculation, shown in appendix B.1, yields
\[
\langle \gamma | \nabla^{2} C|\gamma \rangle = -\frac{8}{2^n} \sum_{x} c(x) \sum_{i \in \ell'} \sin\left(\frac{\gamma}{2} (\partial_{i} \partial_{i'} c(x) + \frac{1}{2} \partial_{i} \partial_{i'} c(x))\right) \sin\left(\frac{\gamma}{2} (\partial_{i} c(x) + \frac{1}{2} \partial_{i} \partial_{i'} c(x))\right),
\]
(62)
which for each \( C_{j} = a_{j}Z_{j_{1}} \ldots Z_{j_{|j|}} \), \( C = \sum_{j} C_{j} \), reduces to
\[
\langle \gamma | \nabla^{2} C_{j}|\gamma \rangle = -\frac{8}{2^{|j|}} \sum_{x \in \{0,1\}^{j}} c_{j}(x) \sum_{i \in \ell'} \sin\left(\frac{\gamma}{2} (\partial_{i} c_{j}(x) + \frac{1}{2} \partial_{i} \partial_{i'} c_{j}(x))\right) \sin\left(\frac{\gamma}{2} (\partial_{i} c_{j}(x) + \frac{1}{2} \partial_{i} \partial_{i'} c_{j}(x))\right).
\]

We apply these results in section 3.3.

3.3. QAOA\( \beta \) with small mixing angle and arbitrary phase angle

In this section we generalize the leading-order QAOA\( \beta \) results of section 3.1 to the case of arbitrary phase angle \( \gamma \), but \(|\beta|\) taken as a small parameter. We show for this regime that QAOA\( \beta \) probabilities and expectation values remain easily expressible in terms of local cost differences, for arbitrary cost functions. Higher order terms may be similarly derived with our framework. (We show complementary results for the setting of small \(|\gamma|\) but arbitrary \( \beta \) in section 3.7 for the case of QUBO cost functions.)

**Theorem 3.3.1.** The probability of measuring each string \( x \) for QAOA\( \beta \) to first order in \( \beta \) is
\[
P_{1}(x) \simeq P_{0}(x) - \frac{2\beta}{2^n} \sum_{j=1}^{n} \sin(\gamma \partial_{j} c(x)),
\]
(63)
and the first-order expectation value is then
\[
\langle C \rangle_{1} \simeq \langle C \rangle_{0} - \frac{2\beta}{2^n} \sum_{j=1}^{n} c(x) \left(\sum_{j=1}^{n} \sin(\gamma \partial_{j} c(x))\right).
\]

Consider a string \( x^{*} \) that maximizes \( c(x) \). Then \( \partial_{j} c(x^{*}) \leq 0 \) for all \( j \). Therefore, assuming \( \gamma > 0 \) is small enough that each product \(|\gamma \partial_{j} c(x^{*})| < \pi \), then we see that the probability of such a state will increase, to lowest order in \( \beta > 0 \). Thus we again see in this regime that to lowest order probability will flow as to increase \( \langle C \rangle \). Similar arguments apply to minimization.
Proof. Expressing $\langle C \rangle_1$ as the expectation value of $U_M(\beta)\overline{C}U_M(\beta)$ as given in equation (27), taken with respect to $|\gamma\rangle := U_p(\gamma)|s\rangle$, gives to low order in $\beta$

$$\langle C \rangle_1 = \langle C \rangle_0 + \beta \langle |\nabla C| \rangle \gamma - \frac{\beta}{2} \langle |\nabla^2 C| \rangle \gamma + \ldots.$$  \hfill (64)

The leading order contribution then follows from equation (60).

Which plugging into equation (64) gives the result for $\langle C \rangle_1$. Similarly, repeating this derivation for the QAOA$_1$ expectation value of $H_x = \langle x| \langle x|$ shows the first-order correction to the probability of measuring each string $x$ is $-\frac{\beta}{2^n} \sum_{j=1}^{n} \sin(\gamma \beta C(x))$ which gives the result for $P_1(x)$.

Applying the small argument approximation $\sin(x) \simeq x$ to theorem 3.3.1 reproduces the results of theorem 2.2.1. Furthermore, extending theorem 3.3.1 to include the second-order contribution in $\beta$ to $\langle C \rangle_1$ follows readily from equations (62) and (64). From analysis similar to the case when both angles are small, and a simple modification to algorithm 1 above it follows that QAOA$_1$ is classically emulatable for sufficiently small $|\beta|$ (up to small additive error), independent of the size of $|\gamma|$.

Corollary 3.3.1. There exists a constant $b$ such that for QAOA$_1$ with $|\beta| \leq b/n$ there is a simple classical randomized algorithm such that for each $x$

$$|P_{\text{class}}(x) - P_1(x)| = O(1/2^n).$$

Proof. The classical algorithm is constructed by adjusting the quantities of algorithm 1 to match those of theorem 3.3.1, which yields identical leading order terms for both algorithms. It remains to bound the error (cf the results and proofs of appendix C.2).

Let $|\gamma\rangle := U_p(\gamma)|s\rangle$. Applying equation (48) to $H_x := |x\rangle\langle x|$ for $P_1(x) = \langle |\gamma\beta|H_x|\gamma\beta\rangle$ gives

$$P_1(x) = P_0(x) + \beta \langle |\nabla H_x| \rangle \gamma + \sum_{j=2}^{\infty} \frac{(i\beta)^j}{j!} \langle |\nabla^j H_x| \rangle \gamma.$$  \hfill (65)

Observe that using $|\langle x| |\gamma\rangle| = \frac{1}{\sqrt{2^n}}$ we have $|\langle \gamma | \nabla^j H_x | \gamma \rangle| \leq (2n)^j |\langle |H_x| |\gamma\rangle| = (2n)^j \frac{1}{2^n}$, so we bound the tail sum as

$$\sum_{j=2}^{\infty} \frac{(i\beta)^j}{j!} \langle |\nabla^j H_x | \rangle \gamma \leq \sum_{j=2}^{\infty} \frac{(2n\beta)^j}{j!} \frac{1}{2^n} \leq \frac{1}{2^n} (e^{2n\beta} - 2n\beta - 1) \leq \frac{2}{2^n} n^2 \beta^2 e^{2n\beta}.$$  \hfill (66)

Thus if $|\beta| = O(1/n)$ this quantity is $O(1/n^2)$ as desired.

Generally, for QAOA with larger parameter values, the leading-order approximations become less accurate as higher-order terms become significant. For large enough parameters, contributing terms will involve cost function differences over increasingly large neighborhoods, and the number of contributing terms may become super-polynomial. Hence the direct mapping to classical randomized algorithms fails to generalize to arbitrary angles as the probability updates will no longer be efficiently computable in general. Indeed, the results of [7] imply that, under commonly believed computational complexity conjectures, there cannot exist an efficient classical algorithms emulating QAOA$_p$ with arbitrary angles in general, even for QAOA$_1$; see remark 3.7.1 below.

In the remainder of section 3 we illustrate the application of our framework by considering several examples including the Hamming ramp toy problem, a simple quench protocol related to QAOA, and QAOA$_1$ for MaxCut and QUBO problems.

3.4. Example: QAOA$_1$ for the Hamming ramp

Here we consider the Hamming weight ramp problem (studied e.g. for QAOA in [23]). We apply our framework to determine the leading order terms of the QAOA$_1$ cost expectation, and show it matches the exact solution.

Consider the Hamming-weight ramp cost function $c(x) = \alpha |x|$ with $\alpha \in \mathbb{R} \setminus \{0\}$ which we may write

$$c(x) = \alpha |x| = \frac{\alpha n}{2} + (\alpha |x| - \frac{\alpha n}{2}) =: \frac{\alpha n}{2} + c_2(x),$$  \hfill (67)

with Hamiltonian

$$C = \frac{\alpha n}{2} I - \frac{\alpha}{2} \sum_j Z_j =: \frac{\alpha n}{2} I + C_Z,$$  \hfill (68)

i.e. $C_Z := -\frac{\alpha}{2} \sum_j Z_j$ represents the function $c_2(x) = \alpha |x| - \frac{\alpha n}{2}$.
3.4.1. Exact results
For QAOA, a simple calculation shows
\[
\langle C \rangle_1 = \frac{\alpha n}{2} + \frac{\alpha n}{2} \sin(\alpha \gamma) \sin(2\beta).
\] (67)
Thus QAOA optimally solves this problem, with probability 1, with angles \( \gamma = \frac{\pi}{2}, \beta = \pi/4 \). Expanding equation (67) using \( \sin(x) = x - \frac{x^3}{3} + \ldots \) gives
\[
\langle C \rangle_1 = \frac{\alpha n}{2} + \alpha^2 n \gamma \beta - \frac{2}{3} \alpha^2 n \gamma \beta ^3 - \frac{1}{6} \alpha^4 n \gamma^3 \beta + \ldots
\] (68)
where the terms not shown are order 6 or higher in \( \alpha \), and \( \gamma, \beta \) combined.

3.4.2. Our framework
Theorems 2.2.1 and 4.2.1 produce the same leading-order expression equation (68) for the Hamming ramp. For this cost function it is easily seen \( d^2c(x) = (-2)^k c_2(x) \), and in particular \( dc(x) = -2c_2(x) = \alpha(n - 2|\alpha|) \) and \( d^2c(x) = 4c_2(x) \). Thus we have
\[
\langle \nabla_c \nabla C \rangle_0 = \frac{2}{2^n} \sum_x c(x) dc(x) = -4 \langle C C_Z \rangle_0 = -4 \sum_j \left( \frac{c_j^2}{4} \right) = -\alpha^2 n
\]
which from theorem 4.2.1 gives the correct leading order contribution \( \alpha^2 n \gamma \beta \). Next we have
\[
\langle \nabla_c \nabla^3 C \rangle_0 = \frac{2}{2^n} \sum_x c(x) d^3c(x) = \frac{8}{2^n} \sum_x c(x) dc(x) = -4 \alpha^2 n
\]
which gives the \( \gamma \beta ^3 \) term coefficient \(-\frac{1}{5} \alpha^2 n \). Next, from lemma 3.6.1 we have \( \nabla^2 C = 4C_Z \), it follows \( \langle \nabla^2_c \nabla^2 C \rangle_0 = 0 \) as anticipated from equation (68). Finally, for the term \( \langle \nabla^3_c \nabla C \rangle_0 \), we have \( \nabla_c \nabla C = \alpha^2 B \) and so
\[
\langle \nabla^3_c \nabla C \rangle_0 = \langle \nabla^2_c \nabla C \rangle_0 = -\alpha^2 \langle \nabla_c \nabla C \rangle = -\alpha^4 \langle B \rangle_0 = -\alpha^4 n.
\]
Using these expressions in theorem 4.2.1 (which generalizes theorem 2.2.1) for QAOA, then gives the correct terms up to 4th order. Figure 4 compares these approximations with the exact behavior.

In [23], variants of the ramp such as the Bush-of-implications and Ramp-with-spike are studied for QAOA, along with cost functions given by perturbations of the ramp. Our techniques similarly apply to these problems. More importantly, theorems 2.2.1 and 4.2.1 may be applied to problems where the exact results are not generally obtainable.

3.5. Example: QAOA for random Max-3-SAT
When applying QAOA to instances drawn from a class of problems, it may be convenient to select a single set of parameters rather than optimizing parameters individually for each instance. For instance, this selection could be QAOA parameters that optimize the average cost for the class of problems. Our framework can address this situation by averaging the cost operators over the class of problems with a fixed choice of parameters.

As an example, here we apply this idea to random Max-3-SAT. A SAT problem in conjunctive normal form consists of \( m \) disjunctive clauses in \( n \) Boolean literals (i.e. variables or their negations). For \( k \)-SAT, each clause involves \( k \) distinct literals. The cost function associated with a Max-\( k \)-SAT instance is the number of clauses an assignment \( x \) satisfies. For Max-3-SAT, the corresponding cost Hamiltonian as in equation (17) and used in lemma 2.5.3 is easily obtained [58]: each clause contributes \( 7/8 \) to \( a_0 \), and \( \pm 1/8 \) each corresponding \( a_i, a_{ij} \) and \( a_{i,j,k} \), with the signs depending on which variables are negated within each clause.

Random \( k \)-SAT instances are constructed by randomly selecting \( k \) distinct variables for each clause and negating each variable with probability one-half. Averaging the squares of the cost coefficients that appear in lemma 2.5.3 over random 3-SAT instances gives
\[
\langle \nabla_c \nabla C \rangle_0 = -\frac{3m}{4}
\] (69)
where here the overline denotes the average over random instances. Applying this in theorem 3.0.1 gives the averaged leading-order change in QAOA expected cost for such random Max-3-SAT instances to be
\[
\langle C \rangle_1 = \langle C \rangle_0 + \frac{3}{4} m \gamma \beta \ldots = \frac{7}{8} m + \frac{3}{4} m \gamma \beta \ldots
\] (70)

...
where \( (C)_0 = \frac{1}{2} m \) corresponds to the expected solution value obtained from uniform random guessing. Similar considerations apply to the higher-order terms of theorem 3.0.1.

An important consideration when using averages over a class of problems is how well they represent the characteristics of typical instances. The variance with respect to instances in the class is one measure of this. As an example, consider random Max-3-SAT with a fixed clause to variable ratio \( m = \alpha n \) as \( n \) increases. This scaling provides a high concentration of hard instances when \( \alpha \) is close to the transition between mostly satisfiable and mostly unsatisfiable instances [73]. In this case, the variance scales as

\[
\text{var}(\langle \nabla_c \nabla C \rangle_0) \sim \frac{9n\alpha^2}{128}.
\]

Thus, the relative deviation in \( \langle \nabla_c \nabla C \rangle_0 \) is proportional to \( 1/\sqrt{n} \). Such concentration indicates that the average leading-order change \( (C)_1 \) is representative of the behavior of individual instances. Thus averaging over the class of problems gives a simple representative expression for how QAOA performs for this class of problems when the angles are small. Similar considerations apply to higher-order terms.

For individual 3-SAT instances, the QAOA parameters can be efficiently evaluated, for example, by extending the prescription of section 3.6 (cf section 4.4). However, for other problem classes, or higher-order terms in the expansion, or QAOA more generally, evaluating such quantities can be challenging. In such cases, averaging over a class of problems can be a simpler proxy for the behavior of typical instances than per-instance evaluation, and, for example, applied toward obtaining good algorithm parameters.

### 3.6. Analysis of QAOA for QUBO problems and MaxCut

Our framework is useful for exact analysis of QAOA with arbitrary angles, not just to leading-order contributions or in small-angle regimes. Such analysis is challenging in general and typically requires some degree of problem specialization. Here we show how our framework may be used to succinctly reproduce analytic performance results previously obtained for MaxCut [14], and extend such analysis to the wider class of QUBO problems. For these problems we have the following.

**Lemma 3.6.1.** For a QUBO cost Hamiltonian \( C = a_0 I + \sum_j a_j Z_j + \sum_{i<j} a_{ij} Z_i Z_j =: a_0 I + C_{(1)} + C_{(2)} \) we have for \( k \in \mathbb{Z}_+ \)

\[
\nabla^{2k} C = 4^k C_{(1)} + 16^{k-1} \nabla^2 C_{(2)},
\]

\[
\nabla^{2k+1} C = 4^k \nabla C_{(1)} + 16^k \nabla^3 C_{(2)}.
\]

We prove the lemma in appendix D. Similar results follow for higher degree cost Hamiltonians (towards analysis of QAOA for problems beyond QUBOs). For example, for a strictly 3-local cost Hamiltonian \( C = \sum_{j<k} a_{ijk} Z_i Z_j Z_k \) it can be shown that any \( \nabla^\ell C \) for \( \ell \geq 4 \) can be expressed as a real linear combination of \( C, \nabla C, \nabla^2 C, \) and \( \nabla^3 C \).

We use lemma 3.6.1 to sum the series \( \sum_{M} C U_M C U_M = C + i\beta \nabla C - \frac{1}{2} \beta^2 \nabla^2 C + \ldots \). Consider an instance of MaxCut, i.e. a graph \( G = (V, E) \) with \( |V| = n \) and \( |E| = m \), with cost Hamiltonian \( C = \frac{m}{2} I - \frac{1}{2} \sum_{(j) \in E} Z_j Z_j \), and the other related operators shown in table 2. From lemma 3.6.1, for a strictly quadratic cost Hamiltonian \( C_Z = \sum_{uv} c_{uv} Z_u Z_v \) we have \( \nabla^{2k+1} C_Z = 16^k \nabla C_Z \) and \( \nabla^{2k} C_Z = 16^{k-1} \nabla^2 C_Z \), where \( \nabla C_Z \) and \( \nabla^2 C_Z \) are easily derived as Pauli operator expansions given in table 2. Hence, it follows \( \sum_{M} C_Z U_M C_Z U_M = C_Z - \frac{1}{2} \sin(4\beta) \nabla^2 C_Z + \nabla C_Z - \frac{1}{2} \sin^2(2\beta) \nabla^3 C_Z \), and applying theorem 3.0.1 for QAOA yields

\[
\langle C \rangle_1 = \langle C \rangle_0 + \frac{\sin(4\beta)}{4} \langle \gamma | \nabla C | \gamma \rangle - \frac{\sin^2(2\beta)}{8} \langle \gamma | \nabla^2 C | \gamma \rangle,
\]

for MaxCut, where \( |\gamma\rangle = U_\beta (\gamma) |s\rangle \) and the angles \( \gamma, \beta \) are arbitrary. (We give a more detailed derivation of equation (74) in appendix D.1.) The right-hand side expectation values depend on the structure of the graph \( G \), as reflected in equations (60) and (62), and may be further reduced. Indeed, we previously computed the quantities of equation (74) for the case of MaxCut in [14, 17] in terms of the proble graph parameters; comparing to [14, theorem 1], we have

\[
\langle \gamma | \nabla C | \gamma \rangle = \sin(\gamma) \sum_{u \in V} d_u \cos^{d_u-1}(\gamma),
\]
where $d_u = \deg(u)$ is the graph degree of vertex $u$, and
\[
\langle \gamma | \nabla^2 C \gamma \rangle = 2 \sum_{(uv) \in E} \cos^{d_u + d_v - 2\omega}_{(uv)} - 2(\gamma) (1 - \cos^{d_v}_{(uv)} (2\gamma)),
\]
(76)
where $f_{uv}$ gives the number of triangles (3-cycles) containing the edge $(uv)$ in $G$. In particular, if $G$ is triangle free then $\langle \gamma | \nabla^2 C \gamma \rangle = 0$. Hence we may always efficiently compute $\langle C_1 \rangle$ for a given instance of MaxCut. Moreover, equations~(74)–(76) lead to QAOA$_1$ performance bounds (i.e. the parameter-optimized expected approximation ratio achieved) for MaxCut for particular classes of graphs; see [14, 17].

Likewise, for general QUBO cost Hamiltonians, applying lemma 3.6.1 yields
\[
\langle C_1 \rangle = \langle C_0 \rangle + \frac{\sin(2\beta)}{2} \langle \gamma | \nabla C_{(1)} \gamma \rangle + \frac{\sin(4\beta)}{4} \langle \gamma | \nabla C_{(2)} \gamma \rangle - \frac{\sin^2(2\beta)}{8} \langle \gamma | \nabla^2 C_{(2)} \gamma \rangle.
\]
(77)
The right-hand side expectation values are independent of $\beta$ and may each be similarly computed as in the case of MaxCut as polynomials of $\gamma$ that reflect the cost Hamiltonian coefficients $a_u$, and underlying adjacency graph, see e.g. [17, appendix E]. Alternatively, they may be computed using equations (60) and (62). Practical computation of these quantities typically takes advantage of linearity of expectation $\langle C_p \rangle = \sum_i \langle C_i \rangle_p$ for cost Hamiltonians $C = \sum_i C_i$ where each $C_i$ is a single weighted Pauli term, as well as problem-locality considerations, as discussed in sections 2.6 and 3.2. Similar formulas for more general problems may be obtained with our framework. As an example we consider a variant of Max-2-SAT.

3.6.1. Example: Analysis of QAOA$_1$ for Balanced-Max-2-SAT

Here we apply our framework to QAOA$_1$ for the Balanced-Max-2-SAT problem, defined as instances of Max-2-SAT such that each variable appears negated or unnegated in an equal number of clauses. Assuming the Unique Games Conjecture in computational complexity theory, there is a sharp threshold $\theta \approx 0.943$ such that it is NP-hard to hard to approximate this problem to $\theta$ or better whereas a $\theta - \epsilon$ approximation can be achieved any polynomial time [74, theorems 3 and 4]; see also [75].\(^{16}\)

Here for simplicity we consider problem instance with the additional assumption that each pair of variables $x_i, x_j$ appears in at most one clause (i.e. one of $x_i \lor x_j$, $\overline{x_i} \lor x_j$, $x_i \lor \overline{x_j}$, or $\overline{x_i} \lor \overline{x_j}$).\(^{17}\) We use $(-1)^{\ell_i j}$ to denote the parity of a given clause, which is $-1$ when only one of $x_i, x_j$ is negated. Then for a Balanced-Max-2-SAT instance with $m$ clauses and $n$ variables, the cost Hamiltonian takes a particularly simple form
\[
C = \frac{3}{4} J - \frac{1}{4} \sum_{(ij) \in E} (-1)^{\ell_i j} Z_i Z_j,
\]
(78)
where we have identified the graph $G = ([n], E)$ with $|E| = m$ edges corresponding to the problem clauses.

For computing $\langle C_1 \rangle = \frac{3}{4} m + \frac{1}{4} \sum_{(ij) \in E} \langle C_i \rangle_1$, the QAOA$_1$-cone of each $C_i$ consists of terms corresponding to edges adjacent to $(ij)$ in $E$. A neighbor $k$ of both $i$ and $j$ defines a triangle in $G$, with parity defined to be the product of its edge parities. Let $F^0$ denote the number of triangles in $G$ with parity $\pm 1$.\(^{18}\) Similarly, for each edge define $f^+ = f^+_{ij}$, $f^- = f^-_{ij}$ with respect to the triangles containing $(ij)$.

Applying our framework and results above (equation (77)), in appendix D.1 we show the exact QAOA$_1$ cost expectation is given as a function of the angles and problem instance by
\[
\langle C_1 \rangle = \langle C_0 \rangle + \frac{\sin(2\beta) \sin(\gamma/2)}{8} \sum_{(ij) \in E} \sum_{\ell=1,3,5,...} \cos^{d+\epsilon-2\gamma} \left( f^+_{ij} \gamma \right) \sin^{d+\epsilon} \left( f^-_{ij} \gamma \right),
\]
\[
\langle C_0 \rangle = \frac{3}{4} m, \quad d_i + 1 \text{ is the degree of vertex } i \text{ in } G, \text{ and we have defined}
\]
\[
g(r^+, r^-; \gamma, \beta) = \sum_{\ell=1,3,5,...} \cos^{2r^+ + 2r^- - \ell \gamma} \left( f^+_{ij} \gamma \right) \sin^{2r^+ + 2r^- - \ell \gamma} \left( f^-_{ij} \gamma \right) \frac{\ell}{\ell} F_1 (\ell).\]
\]
\[16\] A related variant of Max-2-SAT has been previously explored for quantum annealing [76]. In that case, random instances were constructed using equal probabilities of a variable appearing as negated or unnegated in each clause; cf. also section 3.3.
\[17\] We may relax this assumption at the expense of a more complicated proof and presentation of equation (79) due to bookkeeping required, in which case $G$ generalizes to a multigraph.
\[18\] A balanced instance need not have balanced triangles. E.g., the single-triangle instance $x_1 \lor x_2 \lor x_3 \lor x_4 \lor \overline{x_5}$ has $(f^+, f^-) = (0, 1)$ whereas the two-triangle instance $x_1 \lor x_2 \lor x_3 \lor x_4 \lor x_5 \lor x_6 \lor x_7 \lor x_8 \lor x_9$ has $(f^+, f^-) = (2, 0)$. 

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Here \( _2F_1 \) is the Gaussian (ordinary) hypergeometric function; see e.g. [77]. In particular, the function 
\[
\binom{\ell + 1}{\ell} \binom{\ell + 1}{\ell} \binom{-\ell - f^+ - \ell + 1; -1}{\ell}
\] 
occurs in \( g(\cdot) \) evaluates to \( f^+ - f^- \) for \( \ell = 1 \), and to 
\[
\binom{\ell + 1}{\ell} - \binom{\ell + 1}{\ell} = \frac{1}{2} f^+ f^- (f^+ - f^-)
\] 
for \( \ell = 3 \).

Hence for a given Balance Max-2-SAT instance \( (C)_1 \) may be efficiently computed. In some cases we can obtain further simplified expressions. For example, in the case that all triangles in the instance are of the same parity, \( (C)_1 \) is easily seen to reduce to the same formula for MaxCut given in section 3.6 and previously obtained in [14, 17] (up to constant factors and the shift \( \gamma \rightarrow \gamma/2 \) due to the affine mapping between the respective cost Hamiltonians). Indeed, along the way to proving equation (79) in appendix D.1, we rederive equations (74)–(76) using our framework.

Results such as equation (79) may be used to bound the expected QAOA approximation ratio 
\( R_1 = \langle C \rangle_1 / \gamma > \langle C \rangle_1 / m \), where \( \gamma \) is the optimal cost value.

### 3.7. QAOA\(_p\) with small phase angle and arbitrary mixing angle

We conclude section 3 by considering QAOA\(_p\) with small phase angle \( \gamma \) and arbitrary mixing angle \( \beta \) (i.e. the converse case of section 3.3). For simplicity, here we consider QUBO problems as in section 3.6; similar but more complicated formulas follow for more general cost Hamiltonians. We show how the leading order contribution to the cost expectation value reflects cost Hamiltonian structure (Fourier coefficients) of equation (17).

**Theorem 3.7.1.** Consider a QUBO cost Hamiltonian \( C = a_0 I + \sum_i a_i Z_i + \sum_{j<k} a_{jk} Z_i Z_k \). The QAOA\(_p\) expectation value of \( C \) to second order in \( \gamma \) is

\[
\langle C \rangle_1 \approx \langle C \rangle_0 + 2\gamma \left( \sin(2\beta) \sum_j a_j^2 + \sin(4\beta) \sum_{j<k} a_{jk}^2 \right) - 4\gamma^2 \sin^2(2\beta) \sum_{i<j} a_{ij} \left( a_{ai} + \sum_k a_{ak} a_{jk} \right).
\]

**Proof.** Recall \( C(k) \) denotes the Hamiltonian defined as the (sum of the) strictly \( k \)-local terms of \( C = a_0 I + C(1) + C(2) \). Expanding each expectation value in equation (77) to second order in \( \gamma \) and applying lemmas 2.5.1 and 2.5.2 gives

\[
\langle \gamma | i \nabla C(j) | \gamma \rangle = \langle \delta_i \nabla C(j) \rangle_0 - \gamma \langle \nabla C \nabla C(j) \rangle_0 - \frac{\gamma^2}{2} \langle i \nabla^2 \nabla C(j) \rangle_0 + \ldots,
\]

for \( j = 1, 2 \), where \( \langle \nabla C \nabla C(j) \rangle_0 = -4\sum_j a_j^2 \) and \( \langle \nabla C \nabla C(2) \rangle_0 = -8 \sum_{j<k} a_{jk}^2 \) from lemma 2.5.3, which together give the result in the first parenthesis. For the last term in equation (77) we have

\[
\langle \gamma | i \nabla^2 C(j) | \gamma \rangle = \langle \delta_i \nabla^2 C(2) \rangle_0 - \gamma \langle \nabla C \nabla^2 C(2) \rangle_0 - \frac{\gamma^2}{2} \langle i \nabla^2 \nabla^2 C(2) \rangle_0 + \ldots,
\]

with \( \langle \nabla C \nabla^2 C(2) \rangle_0 = 64 \sum_{i<j} a_{ij} a_{ij} + 64 \sum_{i<j} \sum_{k \in \text{nbhd}(i,j)} a_{ik} a_{ij} a_{jk} \) which we show in lemma B.0.2 of appendix B.

**Remark 3.7.1.** The quantities of theorem 3.7.1 may be alternatively expressed in terms of expectation values of classical functions (as in theorem 2.2.1), see lemma B.0.2. However, in contrast to the case of QAOA\(_p\) with small mixing angle considered in theorem 3.3.1, here we do not obtain a simple expression for the the leading order probability of measuring each given \( x \) (i.e. the result of theorem 3.7.1 is not of the form \( \langle C \rangle_1 \approx \sum_x P(x) \langle \gamma \rangle \) for some explicit probability distribution \( P(x) \)). Hence, theorem 3.7.1 does not directly yield a simple classical algorithm approximately emulating QAOA\(_p\) in this parameter regime in the same way as from theorem 2.2.1.

Indeed, a general efficient classical procedure for sampling from QAOA\(_p\) circuits for arbitrary parameters would imply the collapse of the polynomial hierarchy in computational complexity [7], and hence such procedures are believed impossible. Our results are consistent with this viewpoint and indicate that sampling remains hard even as the phase angle becomes small (for constant but sufficiently large mixing angle), but as expected becomes relatively easy when both angles, or only the mixing angle, are sufficiently small. Additional intuition may be gained from the sum-of-paths viewpoint of appendix A.

### 4. Application to QAOA\(_p\)

The gradient operator framework extends to QAOA\(_p\) with arbitrary level \( p \) and parameters \( \gamma_i, \beta_j \). In the Heisenberg picture, the \( j \)th QAOA level acts by conjugating the observable resulting from the preceding \((j + 1)\)th level, in iteration for \( j = p, p - 1, \ldots, 1 \). This approach yields formulas similar to but more general than lemma 3.0.1.
Lemma 4.0.1. The QAOA$\_p$ operator $Q = Q_pQ_{p-1} \ldots Q_2Q_1$, where $Q_i = U_M(\beta_i)U_P(\gamma_i)$, acts by conjugation on the cost Hamiltonian $C$ as

$$Q^\dagger C Q = \sum_{\ell_1} \sum_{k_1=0}^\infty \sum_{\ell_2} \sum_{k_2=0}^\infty \cdots \sum_{\ell_p} \sum_{k_p=0}^\infty (i\gamma_1\nabla_1)^{\ell_1}(i\beta_1)^{k_1}(i\gamma_2\nabla_2)^{\ell_2}(i\beta_2)^{k_2} \cdots (i\gamma_p\nabla_p)^{\ell_p}(i\beta_p)^{k_p} C. \quad (80)$$

The QAOA$\_p$ cost expectation then follows as $\langle C \rangle_p = (Q^\dagger C Q)_0$.

Proof. Follows recursively applying equation (48) for each $Q_j$ as in the proof of lemma 3.0.1.

4.1. Effect of $p$th level of QAOA$\_p$

We next consider the change in cost expectation between a level-$(p-1)$ QAOA circuit (with fixed parameters), and the level-$p$ circuit constructed from adding an additional QAOA level. This case concerns the last layer applied of the QAOA circuit, or, alternatively the effect of an additional layer. The following theorem generalizes theorem 3.0.1.

Theorem 4.1.1. For QAOA$\_p$, the cost expectation satisfies

$$\langle C \rangle_p = \langle C \rangle_{p-1} + \sum_{\ell=0}^\infty \sum_{k=1}^\infty (i\beta_p)^k \langle \nabla_\ell \nabla_k \rangle \langle C \rangle_{p-1}. \quad (81)$$

Here, with respect to the fixed QAOA$\_p$ state $|\gamma\beta\rangle_p$ state, $\langle \gamma\beta \rangle_{p-1}$ indicates the expectation value with respect to the corresponding QAOA$\_p$ state resulting from application of only the first $p-1$ QAOA stages (or, equivalently, $\langle \gamma\beta \rangle$ with $\gamma_p, \beta_p$ set to 0).

Proof. The result follows applying lemma 4.0.1 to the righthand side of $\langle \gamma\beta | C | \gamma\beta \rangle_p = \langle \gamma\beta | \{ Q_p^\dagger C Q_p \} | \gamma\beta \rangle_{p-1}$, where $Q_p := U_M(\beta_p)U_P(\gamma_p)$.

4.1.1. Example: QAOA$\_p$ with small phase and mixing angles at level $p$

When the parameters of the final $p$th level of the QAOA$\_p$ are small, we obtain a generalization of theorem 2.2.1.

Corollary 4.1.1 (Small angles at level $p$). For QAOA$\_p$ with $p$th level angles $\gamma_p, \beta_p$, to second order we have

$$\langle C \rangle_p - \langle C \rangle_{p-1} \simeq \beta_p |i\nabla_C|_{p-1} - \frac{\beta_p^2}{2} \langle \nabla_C^2 \rangle_{p-1} - \gamma_p \beta_p \langle \nabla_C \nabla_C \rangle_{p-1}, \quad (82)$$

where the neglected terms cubic or higher in $\gamma_p, \beta_p$.

Proof. The result follows collecting the quadratic leading-order terms of theorem 4.1.1.

4.1.2. Example: QAOA$\_p$ with small mixing angle at level $p$

We also consider the case of QAOA$\_p$ with small mixing angle $\beta_p$, but arbitrary phase angle $\gamma_p$. This case applies, for instance, in parameter schedules inspired by quantum annealing, where $\beta$ approaches zero at the end of the anneal. The following result generalizes theorem 3.3.1; the proof is similar and is given in appendix B.1.

Corollary 4.1.2. Consider a QAOA$\_p$ state $|\gamma\beta\rangle_{p-1} = \sum_x q_x |x\rangle$ to which another ($p$th) level of QAOA with angles $\beta := \beta_p, \gamma := \gamma_p$ is applied. The change in probability to first order in $\beta$ is

$$P_p(x) - P_{p-1}(x) = -2\beta \sum_{j=1}^n r_{xj} \sin(\alpha_{xj} + \gamma \hat{c}(x)) + \ldots \quad (83)$$

for each $x \in \{0,1\}^n$, where we have defined the real polar variables $r, \alpha$ as $r_{xj} = |q_x|$, $\alpha_{xj} := \arg(q_x) = \arg(e^{-i\alpha_{xj}})$ which reflect the degree of which the coefficients $q_x$ are non-real. The expectation value then changes as

$$\langle C \rangle_p - \langle C \rangle_{p-1} = -2\beta \sum_x \hat{c}(x) \sum_{j=1}^n r_{xj} \sin(\alpha_{xj} + \gamma \hat{c}(x)) + \ldots \quad (84)$$

4.2. Leading-order QAOA$\_p$

When all QAOA angles are small or viewed as expansion parameters, lemma 4.0.1 leads to the following generalization of theorem 3.0.1.

Theorem 4.2.1. For QAOA$\_p$, to fifth order in the angles $\gamma_1, \beta_1, \ldots, \gamma_p, \beta_p$ we have
\[
\langle C_p \rangle = \langle C \rangle_0 - \langle \nabla_c \nabla_c \rangle_0 \sum_{i,j}^{p} \gamma_i \beta_j + \langle \nabla_c \nabla^2 C \rangle_0 \left( \sum_{i,j,k<l} \gamma_i \beta_j \beta_l + \frac{1}{2} \sum_{i,j,k} \gamma_i (\beta_j^2 \beta_k + \beta_j \beta_k^2) + \frac{1}{3!} \sum_{i,j} \gamma_i^3 \beta_j^3 \right)
+ \langle \nabla_c^3 \nabla_c \rangle_0 \left( \sum_{i,j<k<l} \gamma_i \gamma_j \beta_k + \frac{1}{2} \sum_{i<j<k<l} (\gamma_i^2 \gamma_k + \gamma_i \gamma_j \gamma_k) \beta_l + \frac{1}{3!} \sum_{i,j} \gamma_i^3 \beta_j^3 \right)
+ \langle \nabla_c^5 \nabla_c \rangle_0 \left( \sum_{i,j<k<l} \gamma_i \gamma_j \beta_k + \frac{1}{2} \sum_{i<j<k} \gamma_i^2 \beta_k + \frac{1}{2} \sum_{i<j<k} \gamma_i \gamma_j \beta_k^2 + \frac{1}{4} \sum_{i,j} \gamma_i^2 \beta_j^2 + \sum_{i<j<k<l} \gamma_i \beta_j \gamma_k \beta_l \right) + \ldots
\]  

where the terms not shown to the right are each order six or higher in angles and the gradient operator expectations.

The gradient operator initial state expectations of equation (85) are expressed in terms of cost difference functions in equations (42)–(45), and lemma B.0.2 of appendix B. These factors depend only on the cost function. Higher order contributions may be derived similarly.

Remark 4.2.1. Observe that the kth order coefficient of equation (85) consists of sums over products of angles, with each product of degree k. At least one of these sums is indexed by k distinct angles, and the others involve k distinct angles or fewer. Sums with k distinct angles contain a number of terms that scales as \(O(p^k)\) and so these factors dominate when \(p\) becomes large. This observation extends to more general initial states or mixing operators (recalling remark 2.5.1).

Proof. We compute \(\langle C_p \rangle = \langle Q^i C Q \rangle_0\) by taking the expectation value of equation (80) with respect to \(|s\rangle\) and collecting the terms proportional to each cost gradient expectation value. From lemma 2.5.1, only terms for which \(\ell_1 + \ell_2 + \ldots + \ell_p + k_p\) is even can give nonzero contributions. Moreover, from lemma 2.5.2 any expectation value with a leftmost \(\nabla\) or a rightmost \(\nabla_c\) is zero. Applying these rules the only terms which can contribute up to fifth order are

\[
\langle C_p \rangle = \langle C \rangle_0 + a_0 \langle \nabla_c \nabla_c \rangle_0 + a_1 \langle \nabla_c \nabla^3 C \rangle_0 + a_2 \langle \nabla_c^2 \nabla^2 C \rangle_0 + a_3 \langle \nabla_c^3 \nabla C \rangle_0 + a_4 \langle \nabla_c \nabla_c \nabla_c \nabla_c \rangle_0 + \ldots
\]

where the \(a_i\) are real homogeneous polynomials in the angles which correspond to the possible ways of generating its associated gradient operator in the sum equation (80). From lemma 2.5.3 the second order term is \(\langle \nabla_c \nabla_c \rangle_0 = \frac{1}{2} \sum_x c(x) d_c(x)\). The coefficient \(a_0\) follows from each possible selection of the ordered pair \((i \nabla_c)(i' \nabla_c)\) in equation (80) and is easily seen to be \(a_0 = \sum_{i \in \{0\}} \gamma_i \beta_j\). At fourth order, similarly, the coefficients \(a_1, \ldots, a_4\) are degree 4 polynomials and easily calculated as sums corresponding to all possible ways of generating the associated gradient, when the order of each (super)operator product in equation (80) is accounted for. In particular, \(\langle \nabla_c \nabla_c \nabla_c \nabla_c \rangle_0 = \langle \nabla_c^5 \nabla^2 \rangle_0\) from equation (38), which gives \(a_4 = \sum_{i \in \{0\}} \gamma_i \beta_j \) and corresponds to the final term of the last parenthesis.

Repeating the above proof for the QAOA \(P_p(x) = \langle H_x \rangle_p = \langle |x\rangle \langle x|\rangle_p\), as in the proof of theorem 3.0.1 produces the leading-order expression for \(P_p(x)\) given in table 1, and similarly for higher order terms.

Equation (85) shows that for any parameters values the cost function expectation value achieved by QAOA can be expressed as a linear combination of the initial expectation values of \(C\) and its gradients. These expectation values depend only on the structure of the cost function. The dependence on QAOA parameters occurs through the coefficients of each expectation value, which are polynomials of the algorithm parameters. These polynomials are homogeneous but not symmetric. For example, the leading-order coefficient polynomial \(\sum_{i \in \{0\}} \gamma_i^3 \beta_i^3\) depends more strongly on early \(\gamma\) values and late \(\beta\) values, as opposed to late \(\gamma\) values or early \(\beta\) values. Hence equation (85) and its higher-order generalizations may help select parameters. Indeed, for a few-parameter schedule, such as \(\gamma = \gamma_0 + \alpha j\) and \(\beta = \beta_0 + bj\), the coefficients of equation (85) can be computed in terms of the reduced parameter set. In particular, for such linear schedules satisfying \(|\gamma|, |\beta| \leq \Delta\) the leading-order coefficient grows with \(p\) as \(|\sum_{i \in \{0\}} \gamma_i \beta_i^3| = O(\Delta p^3)\).

As an aside we show how the leading-order term of equation (85) yields a simple argument showing that QAOA can also obtain the quadratic quantum speedup for Grover’s problem, reproducing results rigorously obtained in [11]. For convenience consider the case of strings of \(n\) variables with a single marked solution \(x^*\), and corresponding cost Hamiltonian \(C = |x^*\rangle \langle x^*|\). Following [11], we apply QAOA with the standard initial state and mixer, and fixed parameters \(\gamma = \gamma = \pi\) and \(\beta = \beta = \pi/n\), which gives \(\sum_{i \in \{0\}} \gamma_i \beta_i = O(p^2/n)\). In this case the mixing angles become very small as \(n\) becomes large, and hence all
products of phase and mixing angles also become small. Hence, we can reasonably assume that the leading-order term of equation (85) dominates for large \( n \), and neglect the higher-order terms. Since \( \langle C \rangle_0 = 1/2^n \) and \( \langle \nabla C \nabla C \rangle_0 = -2n/2^n \) for this problem, to leading order we have \( \langle C \rangle_p = 1/2^n + O(p^2/2^n) \), where the factors of \( n \) have canceled. Rearranging terms then implies that the success probability \( P_p(x^*) = \langle C \rangle_p = \Theta(1) \) when \( p = \Theta(\sqrt{n}) \), reproducing Grover’s famous speedup for QAOA as obtained in [11]. While this approach does not immediately reveal constant factors or other details, it is particularly useful for obtaining qualitative insights. Beyond Grover’s problem We will apply related ideas using the low-order terms of theorem 4.2.1 to obtain further insights in future work.

We conclude this subsection with two useful remarks.

**Remark 4.2.2.** The included terms of the leading-order coefficient polynomial \( \sum_{1 \leq i < j} \gamma_i \beta_j \) of equation (85) are also illuminated from the following general formulas.

Observe that using \( U_M^\dagger U_M = I \) we have

\[
U_M(\beta) U_p(\gamma) = e^{-i \gamma (U_M(\alpha) C U_M^\dagger(\beta))} U_M(\beta).
\]

Hence for QAOA, with \( Q := U_M(\beta_p) U_p(\gamma_p) \ldots U_M(\beta_1) U_p(\gamma_1) \), we similarly have

\[
Q = e^{-i \gamma_p (U_M(\beta_p) C U_M^\dagger(\beta_p))} \ldots e^{-i \gamma_1 (U_M(\beta_1) C U_M^\dagger(\beta_1))} U_M(\beta)
\]

for \( \beta := \sum_{j=1}^p \beta_j \), where we have used the property \( U_M(\alpha) U_M(\beta) = U_M(\alpha + \beta) \).

**Remark 4.2.3.** To consider QAOA with arbitrary initial states, lemma 4.0.1 may be similarly applied taking expectation values of equation (80) to obtain results analogous to those of theorems 2.2.1, 2.2.2, and 4.2.1. Similar results follow for more general QAOA mixing Hamiltonians under mild conditions. In particular, one only requires the initial state to be an eigenstate of the mixing Hamiltonian for the leading-order term of theorem 4.2.1 to be provably of the same form (as indicated in remark 2.5.1).

**4.2.1. Leading-order QAOA behaves like an effective QAOA.**

Lemma 4.0.1 and theorem 4.2.1 give perturbative expansions in the parameters \( \gamma, \beta_1, \ldots, \gamma_p, \beta_p \), with respect to conjugation by the identity. These results suggest that when all QAOA angles are small in magnitude, only the relatively few nonzero low-order terms will effectively contribute. Hence when all parameters are sufficiently small, QAOA can again be efficiently classically emulated by a similar argument to the \( p = 1 \) case.

**Proof of theorem 2.2.2.** The result follows from theorem 4.2.1 and equation (42). \( \square \)

**Remark 4.2.4.** When all angles are bounded such that \( \gamma, \beta \leq L \), comparing theorem 2.2.2 as \( L \to 0^+ \) to theorem 2.2.1 shows that the cost expectation of QAOA approaches that of an equivalent QAOA, with effective angles \( \gamma', \beta' \) satisfying

\[
\gamma' \beta' = \sum_{1 \leq i < j} \gamma_i \beta_j
\]

Hence as \( L \) becomes small the leading-order term of theorems 2.2.2 and 4.2.1 becomes insensitive to the particular bounded parameter schedule the angles may be derived from.

Hence, when all angles are sufficiently small we may again classically emulate QAOA.

**Remark 4.2.5.** Repeating the analysis of section 3.1.2 we see that for \( p = O(1) \) there exists a sufficiently large polynomial \( q(n) \) such that \( \gamma, \beta \leq 1/q(n) \) then QAOA can be efficiently classically sampled from with absolute error of each probability \( O(1/2^n) \).

**4.2.2. QAOA beats random guessing**

Here we show that QAOA always beats random guessing, in the sense that there always exist polynomially small angles (as opposed to exponentially small) such that \( \langle C \rangle_p \) beats \( \langle C \rangle_0 \) (by a factor at worst polynomially small). The QAOA case implies the same for QAOA. Whereas it is known QAOA beats random guessing for specific problems (cf section 3.6), the following result holds generally.

**Corollary 4.2.1 (QAOA beats random guessing).** Let \( c(x) \) be a cost function on \( n \) bits that we seek to maximize or minimize, with corresponding Hamiltonian \( C. \) Assume \( c \) is nonconstant and \( c(x) \) is bounded by a polynomial in \( n \). Then there exists a polynomial \( q(n) > 0 \) and angles \( \gamma, \beta, \ldots \) that achieve \( \langle C \rangle_p = \langle C \rangle_0 + \Omega(1/q(n)) \) for maximization, or similarly, \( \langle C \rangle_p = \langle C \rangle_0 - \Omega(1/q(n)) \) for minimization.
Proof. Observe as QAOA\(_p\) subsumes QAOA\(_1\) (i.e. by setting \(\gamma_2 = \beta_2 = \cdots = \beta_p = 0\)), it suffices to show the claim for \(p = 1\). Recall from lemma 2.5.3 that \(\langle \nabla C_0 \mid C_0 \rangle_0 < 0\) for nonconstant \(c(x)\), such that the sign of the leading-order contribution in the approximation \(\langle C \rangle_1\) of theorem 2.2.1 (cf. theorem 3.0.1) is equal to the sign of \(\gamma\beta\), and hence the sign of \(\langle C \rangle_1 - \langle C_0 \rangle_0\) can be controlled by selecting the quadrants of \(\gamma, \beta\) appropriately (i.e. for maximization take \(\gamma, \beta > 0\) or \(\gamma, \beta < 0\)). The result then follows observing that we can select sufficiently small \(|\gamma|, |\beta|\) and \(\epsilon\) such that the error bound of corollary 3.1.1 together with the triangular inequality give the result.

Specifically, for simplicity assume we seek to maximize a cost function \(c(x) > 0\); the general case is similar. Let \(a := -\langle \nabla C_0 \mid C_0 \rangle\) which satisfies \(0 < a < 4\pi\|C\|^2\) from lemma 2.5.3, and lemmas C.1.2 and C.1.1 in appendix C.1, and let \(\epsilon = \left(\frac{4}{\pi\|C\|^2}\right)^{1/4}\), \(\gamma = \epsilon^{1/\|C\|^2}\) and \(\beta = \frac{\sqrt{2\pi}}{2}\). Here \(\epsilon\) is selected to satisfy \(\|C\|\epsilon = \frac{1}{2}\gamma\beta a\). These choices satisfy the conditions of corollary 3.1.1 to give \(|\langle C \rangle_1 - \langle C_0 \rangle_0| < \|C\|\epsilon\). Hence \(\langle C \rangle_1 > \langle C \rangle_0\) and the claim follows as

\[
\langle C \rangle_1 - \langle C_0 \rangle_0 = \langle C \rangle_1 - \langle C \rangle_1 + \langle C \rangle_1 - \langle C_0 \rangle_0
\geq -\|C\|\epsilon + \gamma\beta a = \frac{1}{2}\gamma\beta a
= \Omega(1/\text{poly}(n))
\]

where the assumption \(\|C\| = O(\text{poly}(n))\) implies the inverse-polynomial lower bound.

Clearly, the quantities of corollary 4.2.1 may be tightened significantly when considering specific cost functions, or by considering higher-order terms and more involved error bounds.

4.3. Causal cones and locality considerations for QAOA\(_p\)

Here we build off of the definitions and discussion of section 3.2. Suppose again we are given a cost Hamiltonian \(C = a_0 I + \sum_j C_j\) such that each Pauli term \(C_j = a_j Z_{j_1} \cdots Z_{j_{n_j}}\) acts on at most \(|N_j| \leq k\) qubits. Assume each qubit appears in at most \(D\) terms; the causal cone perspective is especially useful when \(D\) is bounded. We let \(L_{j, \ell} \subset [n]\) denote the lightcone of \(C_j\) corresponding to the \(\ell = 1, \ldots, p\) levels of a QAOA\(_p\) circuit applied in turn, with \(L_{j, \ell - 1} \subset L_{j, \ell}\), as defined in table 3. Note that as the QAOA levels act in reverse order with respect to conjugation, each \(L_{j, \ell}\) corresponds to QAOA angles indexed from \(p - \ell + 1, \ldots, p - 1, p\); cf. equation (80). For example, \(L_{j, 1}\) corresponds to the single-level QAOA conjugation of \(C_j\) with angles \(\gamma_p, \beta_p\).

For computing QAOA\(_p\) expectation values such as \(\langle C \rangle_0 = \sum_j \langle C \rangle_j\), each \(\langle C \rangle_j\) may again be computed independently and taking advantage of the QAOA-cones of the \(C_j\). Each \(\langle C \rangle_j\) can be computed by restricting the initial state and resulting operators to at most \(k(\ell + 1 - k)\) qubits, which for particular values may be significantly fewer qubits than \(n\). Moreover, we may apply this idea for each QAOA layer in turn.

Theorem 4.3.1. Let \(C = a_0 I + \sum_j C_j\) be a \(k\)-local cost Hamiltonian (i.e. \(|N_j| \leq k\)), each qubit appears in at most \(D\) of the \(C_j\). Then for QAOA\(_p\) with operator \(Q = Q_p \cdots Q_2 Q_1\), \(Q_\ell = U_{M}(\beta) U_{M}(\gamma)\), we have

\[
\langle C \rangle_0 = \sum_j \langle |0_{L_{j, p}}^{\ell} \rangle |L_{j, p}^{\ell} \rangle C_j \langle L_{j, p}^{\ell} |0_{L_{j, p}}^{\ell} \rangle \otimes L_{j, p}^{\ell}
= \sum_j \langle |0_{L_{j, p}}^{\ell} \rangle |L_{j, p}^{\ell} \rangle Q_1^{p} Q_2^{p-1} \cdots Q_p^{p} C_j Q_p^{p-1} \cdots Q_2^{p} Q_1^{p} |0_{L_{j, p}}^{\ell} \rangle \otimes L_{j, p}^{\ell},
\]

with \(|L_{j, \ell}| \leq \min(k((\ell + 1) - k)\), \(n\)) for \(\ell = 1, \ldots, p\).

The first equality of equation (88) shows that each \(\langle C \rangle_0 = \langle Q_1 C_0 Q_0 \rangle\) can be equivalently computed by discarding from the QAOA\(_p\) circuit any qubits or operators outside of \(L_{j, p}\). The second equality shows that this idea may be applied layerwise, with successive (with respect to conjugation) QAOA layers depending on increasing numbers of qubits. Both properties are relatively straightforward to take advantage of in numerical computations.

Similar results apply for computing QAOA expectation values of a general cost gradient operator as in equation (40) (with respect to the resulting QAOA-cones of its Pauli terms).

Proof. Consider a fixed observable \(C_j = a Z_{j_1} Z_{j_2} \cdots Z_{j_{n_j}}\) for a QAOA\(_p\) circuit. At each \(\ell\)th layer, operators outside of \(L_{j, \ell}\) commute through and cancel with respect to conjugation. Hence applying causality considerations to lemma 4.0.1, in particular the property that mixing operator conjugations cannot increase Pauli term locality, we have
\[ Q^\dagger C Q = \sum_{\ell_1=0}^\infty \sum_{k_1=0}^\infty \cdots \sum_{\ell_p=0}^\infty \sum_{k_p=0}^\infty \sum_{\ell_{p+1}=0}^\infty \sum_{k_{p+1}=0}^\infty \cdots \sum_{\ell_{2p}=0}^\infty \sum_{k_{2p}=0}^\infty \frac{(i\gamma_1 \nabla C)^{\ell_1}(i\beta_1 \nabla)^{k_1} \cdots (i\gamma_p \nabla C)^{\ell_p}(i\beta_p \nabla)^{k_p}}{\ell_1!\ell_2!k_1! \cdots \ell_p!k_p!} C_j \]

\[ = \sum_{\ell_1=0}^\infty \sum_{k_1=0}^\infty \cdots \sum_{\ell_p=0}^\infty \sum_{k_p=0}^\infty (i\gamma_1 \nabla_{\ell_1} C)_{\ell_1}^{j_1}(i\beta_1 \nabla)^{k_1}_{\ell_{p+1}} \cdots (i\gamma_p \nabla C)_{\ell_p}^{j_p}(i\beta_p \nabla)^{k_p}_{\ell_{2p}} C_j, \]

where we recall \( N_j = L_{j,0} \). Taking initial state expectations and summing over \( j \) then gives a slightly tighter result than equation (88). Observing that we may increase each \( L_{j,\ell} \) without affecting expectation values implies the two equalities of equation (88). Finally, the bound on \( |L_{j,\ell}| \) follows similarly observing that each conjugation by \( U_p \) can increase the degree of a given Pauli term by a factor of at most \((D-1)(k-1)\), and that by definition \( |L_{j,\ell}| \leq n \).

### 4.4. Algorithms computing or approximating \( \langle C \rangle_p \)

Here we show two general algorithms for computing QAOA cost expectation values \( \langle C \rangle_p \). The first approach is exact, though its may scale exponentially in \( p \); hence the second approach considers a family of approximations for \( \langle C \rangle_p \) obtained by truncating the series expression of theorem 4.1.1 at a given order. The first approach encompasses much of the existing techniques in the literature. We emphasize that while such classical procedures may be useful, e.g. to help find good algorithm parameters, for optimization applications in general a quantum computer is required to efficiently obtain the corresponding solution samples.

**Algorithm 2.** Compute \( \langle C \rangle_p \) for QAOA\( p \).

1. Input: Parameters \( n, p \in \mathbb{N} \), angles \( (\gamma_1, \beta_1, \ldots, \gamma_p, \beta_p) \in \mathbb{R}^{2p} \), cost Hamiltonian \( C = a_0 I + \sum_{j=1}^m C_j \) with \( m = \text{poly}(n) \) and \( C_j = a_j Z_j \) for \( j \in [n] \).
2. For \( j = 1, \ldots, m \) and \( \ell = 1, \ldots, p \) compute lightcones \( L_{j,\ell} \subseteq [n] \) (or upper bounds).
3. For \( j = 1 \) compute \( Q^\dagger C Q \) as a Pauli sum by restricting the operators in each QAOA level to those in \( L_{j,\ell} \) as in theorem 4.3.1 and its proof.
4. Discard all terms in the sum containing a Y or a Z factor, and set \( \langle C \rangle_p \) as the sum of the remaining coefficients.
5. Apply Steps 3 and 4 for each \( j = 1, \ldots, m \).
6. Return the overall sum \( \langle C \rangle_p = a_0 + \sum_{j=1}^m \langle C_j \rangle_p \).

Algorithm 2 generalizes the proof given in [14, 17] of \( \langle C \rangle_1 \) for MaxCut (equation (74)), and is used, for instance, in [17] to show a similar result for the Directed-MaxCut problem variant. As observed in [3], for \( C = \sum C_j \) the quantities \( \langle C \rangle_1 \) and \( \langle C \rangle_p \) are equal whenever the terms \( C_j \) and \( C_j \) have the same local neighborhood structure with respect to \( p \) and the underlying cost function (more precisely, whenever there exists a permutation of qubits taking \( C_{l_1} \) to \( C_{l_2} \)). This property significantly reduces the number of unique computations of \( \langle C \rangle_p \) required in Steps 3 and 4 in order to compute \( \langle C \rangle_p \), as a recent paper further elaborates [78]. For example, MaxCut on the complete graph it suffices to compute the expectation value for a single edge. Further results concerning symmetry in QAOA are given in [37].

Even for bounded-degree problems, the number of terms involved in computing each \( \langle C \rangle_p \) in algorithm 2 typically grows exponentially with \( p \) which makes exact QAOA performance results difficult to obtain beyond quite small \( p \) in general. Theorems 4.1.1, 4.2.1, and 4.3.1 may be similarly used to obtain faster classical algorithms for approximating \( \langle C \rangle_p \). Given a parameter \( \ell \in \mathbb{N} \), algorithm 3 returns an approximation of \( \langle C \rangle_p \) accurate up to order \( \ell \) in the QAOA angles, such that the accuracy of the returned approximation improves with increased \( \ell \) and converges to the exact value returned by algorithm 2. We describe how worst-case error bounds may be obtained in [84] for fixed truncation \( \ell \) in appendix C.2, though our approximations often perform much better in practice than such bounds may indicate (cf figure 4). We emphasize that the condition \( |\gamma|, |\beta| < 1 \) in optimal parameter sets or restricted parameter schedule parameters often appears in the literature.

Similarly, algorithm 3 may also take advantage of lightcone considerations as in algorithm 2 in computing the quantities \( \langle G_{\alpha} \rangle_0 = \sum \langle G_{\alpha} \rangle_0 \) for \( C = \sum C_j \). For implementation, the set \( \mathcal{A} \) contains at most \( \frac{1}{2} \ell 2^p \) elements and so the operators \( G_{\alpha} \) can be enumerated and efficiently computed as Pauli sums when \( p = O(1) \) and \( \ell = \log n \). If we further restrict to \( \ell = O(1) \), then we can efficiently compute each \( \langle G_{\alpha} \rangle_0 \), and the polynomials \( f_{\alpha}(\gamma_1, \ldots, \beta_p) \) each have \( \text{poly}(n) \) terms. Hence, when \( p, \ell = O(1) \) and the number of terms in \( C \) is \( \text{poly}(n) \), the algorithm can always be implemented efficiently.

Algorithms 2 and 3 may be further combined to yield hybrid approaches to estimating \( \langle C \rangle_p \), where some parameters are treated perturbatively and other exactly, though we do not enumerate these approaches here. We conclude section 4 by considering an alternative approach to deriving series expressions for QAOA quantities.
and the coefficient polynomials $35^518$. Let $\gamma = \ell + \delta$.

Figure 4. Comparison of approximate versus exact approximations of $\langle C \rangle_p$ for QAOA, for the Hamming weight ramp problem $c(x) = \|x\|$. Here we consider the minimization version optimized by the all 0 string. Panel (a) shows the deviation between the exact formula equation (67) and the approximations obtained by restricting equation (68) to 3rd order and 5th order terms, respectively, plotted versus increasing parameter size. The figure also shows a 2, 3-Pade approximation, which is a rational function whose coefficients match the expansion of that function match the 5th order truncated Taylor series [72]. The right panel compares contour plots of $\langle C \rangle_1$ for the indicated angle values. We observe significant overlap between the targeted blue regions of both plots.

Algorithm 3. Approximate $\langle C \rangle_p$ to order $\ell$ in the QAOA angles.

1. Input: Parameters $p, \ell \in \mathbb{N}$, angles $(\gamma_1, \beta_1, \ldots, \gamma_p, \beta_p) \in \mathbb{R}^p$, cost Hamiltonian $C$
2. If $\ell$ is odd then $\ell \leftarrow \ell - 1$.
3. If $\ell = 0$ or $p = 0$ then return $\langle C \rangle_0$.
4. Let $A := \{ (a_1, b_1, \ldots, a_p, b_p) \in \{0, 1, \ldots, \ell - 1\}^p : \sum_j (a_j + b_j) \in \{0, 2, \ldots, \ell\} \}$.
5. Let $G_\alpha = \nabla B_1 \cdots \nabla B_p \Delta^\alpha C$ for each $\alpha \in A$.
6. For each $\alpha \in A$, compute $\langle G_\alpha \rangle_0$ using the lemmas of section 2.5 and the coefficient polynomials $f_\alpha(\gamma_1, \ldots, \beta_p)$ as in the proof of theorem 4.2.1.
7. Return the estimate $\langle C \rangle_p = \sum_{\alpha \in A} f_\alpha(\gamma_1, \ldots, \beta_p) \langle G_\alpha \rangle_0$.

5. Generalized mixers, initial states, and applications

We proposed designs for generalized QAOA mixing Hamiltonians and unitaries in [4,5] beyond the transverse-field Hamiltonian mixer originally proposed in [3]. Such constructions are particularly appealing for optimization problems or encodings with hard constraints. Here we illustrate generalizations of our framework to QAOA constructions for Max Independent Set and a Graph Coloring optimization problems. Similar ideas apply more generally such as to the other optimization problems and corresponding constructions of [5]. We conclude the section with an outline of how the framework may be applied to electronic structure problems of quantum chemistry based on the QAOA construction of [48]. We provide some additional discussion of applications beyond classical optimization in section 6.

For the purpose of this section, consider a general mixing Hamiltonian $B = \sum_j \hat{B}_j$ acting on $n$ qubits with each $[B_j, C] \neq 0$ (and possibly $[B_j, \hat{B}_k] \neq 0$ for some $k \neq j$). We consider here problems such that each $x \in \{0, 1\}^n$ is either feasible, meaning it encodes a valid candidate problem solution, or else infeasible. We assume that the $B_j$ each preserve feasibility, i.e. map the subspace of feasible computational basis states to itself. As the cost Hamiltonian $C$ is diagonal, this immediately implies that the gradients of all orders $\nabla C \cdots \nabla C \Delta B \nabla C$ also preserve the feasible subspace. We show through two examples the relationship between the resulting cost gradients and (generalized) classical cost difference functions. In particular, for Max-Independent-Set we consider the transverse-field mixer augmented with control, and for Graph Coloring problems we consider a type of XY mixer [5,30]. We refer the reader to [5] for additional details and variations.

5.1. Maximum independent set

Consider the NP-hard optimization problem Max-Independent-Set: given a graph $G = (V, E)$ with $|V| = n$ vertices, we seek to find (the size of) the largest subset of independent vertices. Different QAOA variants for this problem were considered in [4–6, 18, 35]; see e.g. [79] for problem details, classical algorithms, and complexity. Proceeding as in [5], we encode subsets of $V$ with $n$ indicator variables $x_j$, which map to $n$-qubit computational basis states $|x\rangle$. The feasible subspace is spanned by the subset of basis states $|x\rangle$, $x \in \{0, 1\}^n$, that encode independent sets (which depend on the particular problem instance). Let $B = \sum_{j=1}^n \hat{B}_j$, where
each $\tilde{B}_j$ is such that $e^{-i\beta \tilde{B}_j} = \Lambda_j(e^{-i\beta X_j})$ is an $X_j$-rotation controlled on all of the neighbors of vertex $j$ not belonging to an independent set $x$, with control function $f_j = \wedge_{\ell \in \text{nbd}(j)} x_\ell$, when which when $f_j(x) = 1$ implies that flipping the $j$th bit of $x$ cannot cause the independent set property to be violated. In [5, 58] we show that

$$\tilde{B}_j = X_j \prod_{\ell \in \text{nbd}(j)} x_\ell$$

suffices, where $x_\ell = \frac{1}{2} I + \frac{i}{2} Z_\ell$ represents the (negation of) the Boolean function returning the $j$th bit of $x$, such when its control function is false $\tilde{B}_j$ acts as the Identity.

Expanding $\tilde{B}_j$ as a Pauli sum, the number of terms in this representation of $\tilde{B}_j$ may be exponential in $n$, for example if $\text{deg}(j) = \Theta(n)$. Nevertheless, each multi-controlled $X_j$-rotation $e^{-i\tilde{B}_j}$ can be efficiently implemented with basic quantum gates [17, 80, 81]. As products of $B_j$ operators connect every feasible state $|x\rangle$ to the empty set state $|00\ldots0\rangle$, it follows [5] that sufficiently many applications of $e^{-i\beta \tilde{B}_j}$ for different $j$ can connect any two feasible solution states $|x\rangle$ and $|y\rangle$. (Note that [5] considers a variety of possible mixing unitaries, constructed, for example, as $e^{-\beta \tilde{B}_j}$ or $\prod e^{-\beta \tilde{B}_j}$, which are inequivalent; we do not deal with this distinction here and focus instead on the classical calculus derived from the $B_j$ generally.)

The mixing Hamiltonians $\tilde{B}_j$ induce a neighborhood structure on the space of feasible solutions, in this case the unit Hamming distance strings that are also feasible. For each $j = 1, \ldots n$ and independent set $x$ we define the local differences

$$\tilde{\partial}c(x):= \begin{cases} \partial c(x) & \text{if } f_j(x) = 1 \\ 0 & \text{else,} \end{cases}$$

i.e. our usual notion of partial difference but restricted to independent sets (feasible strings) connected by single bit flips. Clearly, this structure may be applied to other cost functions over independent sets. For our case of maximizing cardinality, assuming the restriction to feasible states the cost function $c(x) = |x|$ is the Hamming weight of each string, and maps to the Hamiltonian $C = \frac{1}{2} I - \frac{1}{2} \sum_j Z_j$. Hence, observe that each $\tilde{\partial}c(x) \in \{-1, 0, 1\}$. The cost divergence then becomes

$$\tilde{d}c(x) = \sum_j \tilde{\partial}c(x),$$

which is equal to the number of independent sets obtainable from $x$ by flipping a bit from 0 to 1, minus the number obtained flipping a 1 to 0.

The cost gradient becomes

$$\tilde{\nabla}C = [\tilde{B}, C] = \sum_j \nabla \tilde{B}_j C,$$

where the operators $\nabla \tilde{B}_j$ act for each feasible $|x\rangle$ as

$$\nabla \tilde{B}_j C |x\rangle = -\tilde{\partial}c(x)|x(\ell)\rangle.$$

For example, consider the possible choice of initial state $|00\ldots0\rangle$ which encodes the empty set. As all single-vertex sets are also independent, $\tilde{\nabla}C$ acts to give an equal superposition of them as

$$\tilde{\nabla}C |00\ldots0\rangle = -|100\ldots\rangle - |010\ldots\rangle - \cdots - |0\ldots01\rangle.$$

Note that different choices of initial state will lead to different such relations.

Mixed gradients follow similarly. For example, as the cost Hamiltonian is 1-local, it follows $\tilde{\nabla}C = iY_j \otimes \prod_{\ell \in \text{nbd}(j)} x_\ell$, and so we have

$$\nabla c \tilde{\nabla}C = i\tilde{B}.$$
5.2. Graph coloring

Here we consider optimization problems over colorings of a graph. Given a graph \( G = (V,E) \), \(|V| = n \), and \( k \) colors, we say a valid coloring is assignment of a unique color to each vertex, and a proper coloring is a valid assignment such that each edge connect vertices of different colors. Here we assume an arbitrary cost function \( c(y) \) we seek to optimize over valid colorings \( y \). For example, the Max-\( k \)-Cut generalization of MaxCut is the maximization problem where \( c(y) \) gives the number of edges with different colors. Several other NP-hard variants of optimization problems over valid or proper graph colorings are considered in [5].

Generally, depending on \( k \) and the qubit encoding used, some bitstrings may represent invalid colorings. Following [5, 30] we consider encoding the coloring of each vertex using the Hamming weight-1 subspace of \( k \) qubits, for \( kn \) qubits total. (This encoding may be equivalently viewed as \( n k \)-dits [5], which we utilize below.) Valid vertex colorings then span a \( k^n \)-dimensional subspace of the \( 2^kn \)-dimensional Hilbert space, with proper colorings corresponding to a subspace that depends on \( G \). Hence we may write computational basis states encoding valid (or proper) colorings as \( |y⟩ = |y_1 y_2 \cdots y_n⟩, y_j ∈ [k] \).

A natural mixer for this encoding is the ring \( XY \)-mixer [5, 30] derived from the Hamiltonian

\[
\tilde{B} := \sum_{j=1}^n \tilde{B}_j
\]

where \((j, \ell)\) labels the qubit encoding the \( \ell \)th color variable for the \( j \)th vertex and the label additions are modulo \( k \). (Here the factor of \( 1/2 \) is included for convenience.) We may identify left- and right-shift operators \( L_j,R_j \) which act as

\[
L_j|y⟩ = |y_1 \cdots y_{j-1}(y_j - 1)y_{j+1} \cdots y_n⟩ = |y^{(j,-1)}⟩,
\]

with \( L_j^2|y⟩ = L_jL_j \cdots L_j|y⟩ = |y^{(j,-\ell)}⟩ \), and

\[
R_j|y⟩ = |y_1 \cdots y_{j-1}(y_j + 1)y_{j+1} \cdots y_n⟩ = |y^{(j,+1)}⟩,
\]

with \( R_j^2|y⟩ = |y^{(j,\ell)}⟩ \). As in [5, appendix C] we may write

\[
\tilde{B}_j = L_j + R_j,
\]

Hence in this case, from the structure of the mixing Hamiltonians, for a generic cost function \( c(y) \) we define left and right \( j \)th partial differences

\[
\partial_{j,L}c(y) := c(y^{(j,-1)}) - c(y),
\]

\[
\partial_{j,R}c(y) := c(y^{(j,+1)}) - c(y).
\]

These functions relate to the action of the generalized partial gradients

\[
∇_{\tilde{B}}C|y⟩ = - \langle \partial_{j,L}c(y)L_j + \partial_{j,R}c(y)R_j |y⟩
\]

and hence we have

\[
\tilde{∇}C = - \sum_j (L_j\partial_{j,L}C + R_j\partial_{j,R}C).
\]

Thus in this case we see that the gradient corresponds to cost differences with respect to left and right shift of each \( k \)-dit variable.

The Hamiltonians \( \tilde{B}_j, \tilde{B} \) together with the diagonal cost Hamiltonian \( C \) and their derived gradients have the important property of mapping valid colorings to valid colorings. This property is preserved if we replace the ring structure of the sum in equation (89) with a fully connected one, i.e.

\[
\tilde{B}_j = \sum_{\ell < m} X_{j,\ell}X_{j,m} + Y_{j,\ell}Y_{j,m}
\]

in which case the above expressions generalize to shifts in \( k \)-many directions. This property is maintained if we instead consider sequential mixers \( U(β) = \prod U_i(β) \) built from partial mixers \( U_i(β) = e^{-iβ2\sum e^{j_kx_k}z_{k,m}} \), in
which case the order of the $U_i$ becomes important due to noncommutativity [5] and this will be reflected when applying our framework.

Finally, these QAOA constructions, and our framework, extend to problems where we seek to restrict to proper graph colorings by combining the $XY$ mixers here with control, analogous to the controlled transverse-field mixers for Max-Independent-Set [5].

5.3. Electronic structure

Here we outline how our framework may be applied to problems beyond combinatorial optimization, in particular the prototypical electronic structure problem of quantum chemistry. A recent work [48] proposed and studied a generalization of QAOA suitable for this problem, and we follow this approach here. This application demonstrates the breadth of our framework and how it may be applied to diverse problems and ansätze. Indeed a wide variety of different ansätze have been proposed for this problem, see for example [48, 82].

Consider an instance of the electronic structure problem corresponding to an electronic Hamiltonian $C$ given in second quantized form, specified as a quartic polynomial of fermionic creation and annihilation operators with respect to a truncated single-particle basis, for which we seek to find its ground state and energy $E_0$; see [48, 82] and references therein for the technical details. For such problems it is standard to assume that one has classically obtained the Hartree–Fock approximate ground state and energy $E_{0, HF}$, and has suitably rotated the operators (orbitals) such that the Hartree–Fock ground state is encoded on the quantum computer by a single computational basis state $|HF\rangle$, which we take as the QAOA initial state.

Identifying $C$ as the cost Hamiltonian, a natural choice of mixer is then derived from the Hartree–Fock approximation as

$$B = E_{0, HF}|HF\rangle\langle HF| + \ldots$$

where the terms not shown to the right similarly correspond to the excited states and energies of the Hartree–Fock approximation (i.e. are generated from the possible excitations of the Hartree orbitals). With this choice, the resulting QAOA circuits retain the desirable property of reproducing adiabatic quantum annealing behavior in particular limits as the QAOA depth $p$ becomes large. However, we note that, in contrast to the usual QAOA operators, here the mixing Hamiltonian is diagonal with respect to the computational basis while the cost Hamiltonian is not. Also observe that this QAOA construction satisfies the properties of remark 2.5.1 and so many of our results apply immediately in this setting.

In particular, the main focus of [48] is regimes where $p$ is relatively large, and phase and mixing angles are drawn from a fixed schedule such that their magnitudes are relatively small. Hence we jump straight to the generalization of theorem 4.2.1. For QAOA$_p$ it then follows that to leading-order we have

$$\langle C \rangle_p = \langle C \rangle_0 - \langle \nabla C \nabla C \rangle_0 \sum_{1 \leq i < j} \gamma_{ij} \beta_j + \ldots$$

$$= E_{0, HF} + 2(E_{0, HF} \langle \phi | \phi \rangle - \langle \phi | B | \phi \rangle) \sum_{1 \leq i < j} \gamma_{ij} \beta_j + \ldots,$$

where the terms not shown the the right are again proportional to higher-order polynomials in the angles. The second line follows using $|\phi\rangle := C|HF\rangle$, and using standard properties of Hartree–Fock approximations it follows that $E_{0, HF} \langle \phi | \phi \rangle - \langle \phi | B | \phi \rangle \leq 0$. This last property shows that, for positive angles, to leading order the QAOA ground state energy estimate is guaranteed to improve upon the Hartree–Fock estimate.

Further analysis may be applied in the spirit of our results obtained for combinatorial optimization. In particular, in future work we will leverage this generalization of the framework to help explain universal behavior empirically observed in QAOA performance (phase) diagrams across different problems and settings in [48]. Finally, we remark that the underlying approach and analysis of our framework is relatively straightforward to extend to particular ansätze beyond QAOA, such as the UCC-SD (unitary coupled cluster singles and doubles) ansatz considered in [82].

6. Discussion and future directions

Our framework provides tools for, and its application provides new insights into, layered quantum algorithms. We focused on our framework’s application to QAOA circuits. Specifically, we used it to obtain both new results and more succinct ways of expressing and seeing existing results for transverse field QAOA$_p$,
for general $p$, not just $p = 1$. We also discussed two examples of our framework applied to QAOA with more complicated mixing operators.

Our framework applies more broadly than just the cases discussed in this paper, providing a promising approach to obtain both additional results for QAOA and insights into other types of problems and quantum algorithms.

For example, the framework can be applied to eigenvalue problems related to physical systems. For instance, the general conjugation formula equation (48) has been previously invoked [82, section I] in the context of particular parameterized quantum circuits for the electronic structure problem of quantum chemistry. Similar to but more general than the quantum alternating operator ansatz approach of [48] considered in section 5.3, circuit ansätze for this problem are often built from fermionic creation and annihilation operators and simple reference (e.g. Hartree–Fock) initial states. These operators then have natural interpretations in terms of transitions between occupied orbitals, analogous to the operator-function correspondence of section 1.1, suggesting a route for future work to apply and extend our framework and results in detail to different ansätze for this setting.

For QAOA and beyond, questions related to parameter setting may be amenable to the series approaches of our framework, in particular toward a better understanding of parameter concentration and landscape independence phenomena, as well as implications for algorithm performance limitations [21, 33, 45, 46]. Moreover our framework may be applied in both in ideal and realistic (noisy) settings. For example, in cases when noise largely flattens the cost expectation landscape [34, 83], our series expressions with only a few terms may be sufficient to capture key aspects of the behavior.

In addition to further applications to QAOA, our framework can give insights into recently proposed variants such as adaptive QAOA [54] and recursive QAOA [33]. The framework and obtained results could also provide insight into quantum annealing (QA) and adiabatic quantum computing (AQC) given the close ties between parameters for QA and QA or AQC schedules [19, 48–51], including to cases with advanced drivers [84–86]. One such application of our formalism is designing more effective mixing operators and ansätze, and facilitating quantitative means for comparing them. Our framework suggests direct approaches to incorporating cost function information into mixing operators, such as, for example, using $\nabla C$ as a mixing Hamiltonian. Indeed, the ansatz $U(\alpha) |s\rangle = e^{-i\alpha \nabla C} |s\rangle$ has the same leading-order contribution to $\langle C \rangle$ as QAOA, suggesting a route for future work to apply and extend our framework and results in detail to different ansätze for this setting.

As a practical matter, evaluating series approximations derived from our framework is straightforward but can become tedious when one desires to include many terms. In these situations, computer algebra systems or numerical software can readily compute the required expressions. Moreover, manipulating the resulting series can improve the accuracy for a fixed number of terms. For example, instead of truncating the series expansion at a finite number of terms, giving a polynomial approximation, often better numerical approximations arise from Padé approximants, which are rational functions whose coefficients match the truncated Taylor series [72] (cf figure 4).

These potential applications of our formalism highlight its general applicability to understanding algorithms based on layered quantum circuits, including identifying new operators and ansätze matched to the structure of specific problems.

Data availability statement

All data that support the findings of this study are included within the article (and any supplementary files).

Acknowledgments

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Appendix A. Sum-of-paths perspective for QAOA

Here we briefly show how QAOA probabilities (and similarly cost expectation values) can be expressed as sums over sequences of bitstrings (‘paths’), each weighted by functions of the Hamming distances and cost function values along the path. This ‘sum-of-paths’ perspective complements the main results of our framework and provides additional intuition, though the resulting expressions are no longer power series in the algorithm parameters. Indeed several results of the paper were originally derived using a sum-of-paths approach, but with significantly more complicated proofs than those obtained with our QAOA framework; on the other hand, some tasks are convenient in the sum-of-paths formulation such as working directly with QAOA state amplitudes.

Consider the QAOA mixing operator matrix elements \( u_{d(x,y)}(\beta) = \langle x| U_M(\beta)|y \rangle = \cos^p(\beta)(-i\tan\beta)^d(x,y) \) given in equation (6) for Hamming distance \( d(x,y) \), which satisfy \( u_{ij}^d = (-1)^d u_{ij} \). For QAOA, using the computational basis decomposition \( I = \sum_y |y\rangle \langle y| \) the probability amplitude corresponding to each string \( x \in \{0,1\}^n \) is

\[
\langle x|\gamma\beta \rangle = \sum_y \langle x| U_M(\beta)|y \rangle \langle y| U_P(\gamma)|s \rangle = \frac{1}{\sqrt{2^n}} \sum_y u_{d(x,y)}(\beta)e^{-i\gamma c(y)},
\]

i.e. the amplitude \( \langle x|\gamma\beta \rangle \) may be expressed as sum of ‘single-step paths’ (from each possible \( y \in \{0,1\}^n \), to \( x \)) with each path contributing \( u_{d(x,y)}(\beta)e^{-i\gamma c(y)} \) times its initial amplitude \( \langle y|s \rangle = 1/\sqrt{2^n} \). The probability \( P_i(x) = |\langle x|\gamma\beta \rangle|^2 \) of measuring \( x \) is then

\[
P_i(x) = \frac{1}{2^n} \sum_{y,x} u_{d(x,y)}^* u_{d(x,y)} e^{-i\gamma(c(y)-c(z))}
= \frac{1}{2^n} \sum_{y,z} \cos^{2n}\beta (\tan\beta)^d(x,y) \cos\gamma c(y) - \cos\gamma c(z) d(x,y) e^{-i\gamma(c(y)-c(z))}
= \frac{\cos^{2n}\beta}{2^n} \left( \sum_{d(x,y)=d(x,y)\text{even}} (\tan\beta)^d(x,y) \cos\gamma c(y) - \cos\gamma c(z) d(x,y) \right)
+ \sum_{d(x,y)=d(x,y)\text{odd}} (\tan\beta)^d(x,y) (-1)^{d(x,y)-d(x,z)-1} \sin\gamma(c(y)-c(z))
\]

where the last equation follows because \( \cos \) and \( \sin \) are even and odd functions, respectively, and shows explicitly that all contributing terms are real valued, but with differing signs that may lead to term cancellation (i.e. paths may ‘interfere’). The signs depend on the algorithm parameters, the difference in cost function between \( y \) and \( z \), and their Hamming distances of from \( x \).

Thus we see that the probability \( P_i(x) \) corresponds to a sum of two-step paths (\( z \) to \( x \) to \( y \)) with weights as shown in equation (92). The cost expectation \( \langle C \rangle = \sum_x c(x) P_i(x) \) then follows from additionally weighting all paths in \( P_i(x) \) by \( c(x) \), and then summing over all \( x \in \{0,1\} \). Furthermore, Taylor expansions of equation (92) reproduce the leading-order contributions of theorem 2.2.1, though with considerably more effort than required for our proof.

It is straightforward to extend the sum-of-paths perspective to QAOA\(_p\) with \( p \geq 1 \), at the expense of additional notation. In this case probabilities correspond to paths of length \( 2p \). Let \( u_{d(x,z)}^{(p)} := u_{d(x,z)}(\gamma,\beta) \), and let \( Q_i(x) \) denote the amplitude of computational basis state \( |x \rangle \) after \( j \) layers of QAOA have been applied. Clearly, \( Q_0(x) = 1/\sqrt{2^n} \), and \( Q_i(x) = \langle x|\gamma\beta \rangle \) is given in equation (91). Generalizing equation (91) for a QAOA\(_p\) state gives

\[
Q_p(x) = \sum_{z} u_{d(x,z)}^{(p)} e^{-i\gamma p c(z)} Q_{p-1}(z),
\]

which may be expanded recursively to give

\[
Q_p(x) = \frac{1}{\sqrt{2^n}} \sum_{z_1,z_2,\ldots,z_p} u_{d(z_1,z_2)}^{(1)} u_{d(z_2,z_3)}^{(2)} \cdots u_{d(z_p,x)}^{(p)} e^{-i\gamma c(z_1)+\gamma c(z_2)+\cdots+\gamma c(z_p)}.
\]
Hence computational basis amplitudes after \( p \) levels of QAOA are likewise given by paths consisting of \( p \)-tuples of intermediate bitstrings, weighted by phase factors corresponding to cost function evaluations and mixing matrix elements corresponding to Hamming weight differences along the path.

Expressions for the probability and expected cost may then be obtained from \( P_p(x) = |Q_p(x)|^2 = Q_p^*(x)Q_p(x) \) as above. While in principle this approach can also lead to results such as theorem 2.2.2, our proof provides a more succinct route. Nevertheless, the sum-of-paths perspective gives a different but complementary perspective into QAOA, and the general approach outlined here may be extended to a wider variety of ansätze, such as QAOA with generalized mixers, encodings, and initial states.

**Appendix B. Initial state expectation values**

Here we extend the results of section 2.5. For a linear operator \( A \) on \( n \) qubits we write its computational basis representation \( A = \sum_{x,y} a_{xy} |x⟩⟨y| \) with matrix elements \( a_{xy} := ⟨x|A|y⟩ \in \mathbb{C} \) for \( x, y \in \{0, 1\}^n \). The operator \( A \) is traceless if and only if \( \sum_x a_{xx} = 0 \).

**Lemma B.0.1.** Let \( C \) be a cost Hamiltonian and \( A \) a cost gradient as in (40) such that \([A, C] \neq 0\) and \( A|s⟩ = \frac{1}{\sqrt{2^n}} \sum_x g(x)|x⟩ \) for a real function \( g(x) \).

Then there exists a real function \( g(x) \) satisfying \( \nabla C A|s⟩ = \frac{1}{\sqrt{2^n}} \sum_x \nabla C g(x)|x⟩ \), and:

- If \( A \) is skew-adjoint \( A^† = -A \) then \( \sum_x a(x) = 0 \),

  \[ \langle \nabla C A⟩_0 = \frac{2}{2^n} \sum_x c(x) a(x) = \frac{1}{2^n} \sum_x g(x), \quad \text{and} \quad \langle \nabla C^2 A⟩_0 = 0. \]

- Else if instead \( A \) is self-adjoint \( A^† = A \) then \( \langle \nabla C A⟩_0 = \sum_x g(x) = 0 \), and

  \[ \langle \nabla C^2 A⟩_0 = \frac{1}{2^n} \sum_{x \neq y} (c(x) - c(y))^2 a_{xy} = \frac{2}{2^n} \sum_x c(x) g(x) \]

  \[ = \frac{2}{2^n} \sum_x c^2(x) a(x) - \frac{2}{2^n} \sum_{x, y} c(x) c(y) a_{xy}. \]

The condition \([A, C] \neq 0\) is included because otherwise trivially \( \nabla C A = \nabla C^2 A = 0 \) and so the quantities of the lemma become identically zero. Recall a cost gradient \( A \) may be uniquely decomposed into its diagonal and off-diagonal parts \( A = A_{\text{diag}} + A' \) with respect to the computational basis, with \( \nabla C A = \nabla C A' \). As the results of the self-adjoint case are invariant under replacing \( A \) by \( A + E \) for a traceless real diagonal matrix \( E \) (such that \( \nabla C E = 0 \)), we can replace \( a(x) \) above by any function \( a(x) + c(x) \) where \( \sum_x c(x) = 0 \); hence we can often ignore any diagonal component of cost gradient operators in computing initial state expectation values.

**Proof.** From the definition of \( A \) we have \( a(x) = \sum_y a_{xy} \) and \( a_{xx} = \pm a_{xy} \) when \( A^† = \pm A \), which implies \( \sum_y a(x) = 0 \) when \( A^† = -A \). Using \( A = \sum_{x,y} a_{xy} |x⟩⟨y| \), the function \( g \) is defined as \( \frac{1}{\sqrt{2^n}} g(x) := ⟨x|\nabla C A|s⟩ \) and satisfies

\[ \frac{1}{\sqrt{2^n}} g(x) = ⟨x|CA - AC|s⟩ = \frac{1}{2^n} \sum_y c(y) a(x) - \frac{1}{2^n} \sum_y c(y) a_{xy} = \frac{1}{2^n} \sum_y a_{xy} (c(x) - c(y)), \]

which implies \( \sum_y g(x) = 0 \) when \( A^† = A \). Indeed, from \( ⟨s|A = \frac{1}{\sqrt{2^n}} \sum_y a(x) |s⟩ \) we have

\[ \langle g|_0 = \langle s|\nabla C A|s⟩ = \langle s|CA|s⟩ - \langle s|AC|s⟩ = ⟨0|0⟩ + ⟨0|0⟩ \]

when \( A^† = \pm A \), which shows the results for \( \langle \nabla C A⟩_0 \). Similarly, \( ⟨s|\nabla C A = \frac{1}{\sqrt{2^n}} \sum_x g(x) |x⟩ \) and so

\[ \langle s|\nabla C^2 A|s⟩ = \langle s|C \nabla C A|s⟩ - \langle s|\nabla C A C|s⟩ = \langle g|_0 ± \langle g|_0 \]

\[ = \langle s|C^2 A - 2CAC + AC^2|s⟩ = \langle c^2|_0 ± \langle c^2|_0 - 2\langleCAC|_0. \]

Finally, we use \( \langle c^2|_0 = \frac{1}{2^n} \sum_x c^2(x) a(x) = \frac{1}{2^n} \sum_{x,y} \frac{1}{2^n} c^2(x) a_{xy} \) and \( \langle CAC|_0 = \frac{1}{2^n} \sum_{x,y} c(x)c(y) a_{xy} \) for the case \( A = A^† \) to give

\[ \langle \nabla C^2 A⟩_0 = \frac{2}{2^n} \sum_{x,y} (c^2(x) - c(x)c(y)) a_{xy} = \frac{1}{2^n} \sum_{x,y} (c^2(x) + (2c(x)c(y)) a_{xy} \]

which shows the terms in the sum with \( x = y \) are zero and implies that last equation of the lemma. \( \square \)
We use the lemma to prove equations (43)–(45) concerning the nonzero initial state expectation values of cost gradient at fourth order. The technique of the proof may be used to similarly compute higher order expectation values.

**Lemma B.0.2.** For a cost Hamiltonian $C$ representing real function $c(x)$ we have:

- $\langle \nabla_c \nabla^3 C \rangle_0 = \frac{2}{N} \sum_x c(x) d^3 c(x)$
- $\langle \nabla_c \nabla^2 C \rangle_0 = \frac{2}{N} \sum_{x,k} \langle \partial c(x) \rangle^2 \partial_k c(x)$
- $\langle \nabla_c \nabla C \rangle_0 = \frac{2}{N} \sum_x c(x) \partial_j (\partial c(x))^3 = -\frac{1}{2} \sum_{x,k} \langle \partial_j c(x) \rangle^4$

where $\partial_j c(x) := c(x^{(j)}) - c(x) = \partial_j \partial_k c(x) + \partial_j c(x) + \partial_k c(x)$.

In particular, for a QUBO cost Hamiltonian $C = a_0 + \sum_j a_j Z_j + \sum_{i<j} a_{ij} Z_i Z_j$ these quantities can be further expressed (defining $a_{ij} := a_{ij}$) as:

- $\langle \nabla_c \nabla^3 C \rangle_0 = -16 \sum_i a_i^2 - 128 \sum_{i<j} a_{ij}^2$
- $\langle \nabla_c \nabla^2 C \rangle_0 = 64 \sum_{i<j} a_i a_j + 192 \sum_{i<j<k} a_{ij} a_{jk} a_{ik}$
- $\langle \nabla_c \nabla C \rangle_0 = -16 \sum_i a_i^2 - 32 \sum_{i<j} a_{ij}^2 - 96 \sum_{i<j<k} a_{ji}^2 (a_{jk}^2 + a_{kj}^2 + \frac{1}{2} \sum_{k\neq j,l} (a_{kl}^2 + a_{lk}^2))$

The second part of the lemma shows that we may always efficiently compute the quantities of the first part for cost functions such as QUBOs. Moreover, each expectation values reflects the topology of the underlying QUBO problem graph; for example, for MaxCut, $\langle \nabla_c \nabla^2 C \rangle_0$ is seen to be identically zero on triangle-free graphs.

**Proof.** Recall that any diagonal part of $A$ in lemma B.0.1 can be ignored (such as, for example, in $\nabla^2 C$ for MaxCut from table 2) as it will not affect the initial state expectation values.

The first result follows from the first case of lemma B.0.1 with $A = \nabla^3 C = -A^\dagger$ which from (32) satisfies $a(x) = d^3 c(x)$ to give $\langle \nabla_c A \rangle_0 = \frac{2}{N} \sum_x c(x) d^3 c(x)$. The second result follows applying the second case of lemma B.0.1 to $A$ defined as the non-diagonal part of $\nabla^2 C$, which from (29) has matrix elements $a_{ij} = 2\partial_j \partial_k c(x) = 2\partial_j \partial_k c(x^{(j)})$ when $x$ and $y = x^{(j)}$ differ by two bit flips $j, k$, and $a_{ij} = 0$ otherwise, and so

$\langle \nabla_c \nabla^2 C \rangle_0 = \frac{2}{N} \sum_x \sum_{i<j} (c(x) - c(x^{(j)}))^2 \partial_i \partial_j c(x)$,

where $c(x^{(j)}) - c(x) = \partial_j \partial_k c(x) + \partial_j c(x) + \partial_k c(x)$ follow from the definitions of section 2.1. Additionally, from the Jacobi identity and (38) we have $\langle \nabla_c \nabla \nabla^2 C \rangle_0 = \langle \nabla_c \nabla^2 C \rangle_0$. For the third result, let $A = \nabla_c \nabla C = A^\dagger$, for which from (34) we have $a_{ij} = -(\partial c(x)^3)$ when $y = x^{(j)}$ and $0$ otherwise, and hence the first equality of the second case of lemma B.0.1 gives $\langle \nabla_c A \rangle_0 = \frac{2}{N} \sum_x \sum_{i<j} c(x) (c(x) - c(x^{(j)}))^2 (-\partial c(x)^3)^2 = -\frac{1}{2} \sum_x \sum_{i<j} (\partial c(x))^4$.

This sum can be easily rearranged to become $\frac{2}{N} \sum_x \sum_{i<j} c(x) \partial_i (\partial c(x))^3$, or alternatively this may be obtained from the second equality of the second case of lemma B.0.1 by defining the function $g(x) = (\partial c(x)^3)^3$ from (36) that corresponds to $\nabla_c A$.

Now further suppose we have a QUBO cost Hamiltonian $C := a_0 I + C_1 + C_2$. We proceed by expanding each cost gradient as a linear combination of Pauli operators, and then computing the initial state expectation value using the observation that only terms containing stricly $I$ or $X$ factors can contribute (see [17, section YY] for details). Note that this approach allows us to avoid dealing with exactly computing the coefficients of various terms which cannot contribute.

Let $C_{2, Y} := \sum_{i<j} a_{ij} Y_i Y_j$ and here we write $a_{ij} = a_{ji}$, $a_{ij} := 0$, and $j \in nbd(i)$ if $a_{ij} \neq 0$. Applying lemma 3.6.1 and the Pauli matrix commutation relations ([X, Y] = 2iZ and cyclic permutations) we have $\nabla C = \nabla C_1 + \nabla C_2$, $\nabla^2 C = 4C_1 + 8C_2$, and $\nabla^3 C = 4\nabla C_1 + 16\nabla C_2$. Hence $\nabla_c \nabla^3 C = -16 \sum_i a_i^2 X_i - 64 \sum_{i<j} a_{ij}^2 (X_i + X_j) + \ldots$ where the terms not shown to the right each contain $Z$ factors (for example, terms proportional to $a_{ij} a_{ij} X_j Z_j$), which implies $\langle \nabla_c \nabla^3 C \rangle_0 = -16 \sum_i a_i^2 - 128 \sum_{i<j} a_{ij}^2$ as stated.

Similarly, $\nabla_c \nabla^2 C = -8\nabla C_2$, $\nabla_c \nabla C = 16 \sum_{i<j} a_{ij} (a_{ij} X_i Y_j + a_{ij} Y_i X_j + \sum_{k\neq i,j} (a_{ik} Z_i Y_j + a_{ij} Y_i X_k))$, and so $\nabla_c \nabla^2 C = 64 \sum_{i<j} a_{ij} a_{ij} a_{ij} X_i X_j + 64 \sum_{i<j} a_{ij} a_{ij} a_{ij} X_i X_j + \ldots$ with the terms to the right each containing $Y$ or $Z$ factors. As $a_{ij} = 0$ the $a_{ij} a_{ij} a_{ij}$ terms are nonzero only for triangles in the graph formed from nonzero $a_{ij}$ which implies $\langle \nabla_c \nabla^2 C \rangle_0 = 64 \sum_{i<j} a_{ij} a_{ij} a_{ij} + 3 \sum_{i<j<k} a_{ij} a_{ij} a_{ij} a_{ij} a_{ij}$.

Finally, a similar calculation for gives the result for $\langle \nabla_c \nabla C \rangle_0$, as can readily be seen expanding the identity $\nabla_c \nabla C = \nabla_c^2 B$. □
B.1. QAOA with small mixing angle

Here we show two proofs related to results in sections 3.2, 3.3, and 4.1.2.

**Proof of equation (62).** Recal the notation $\nabla = \sum_i \nabla_i$ with $\nabla_i = [X_i, \cdot]$. As for any $C$

$$\nabla^2 C = \sum_i \nabla_i^2 C + 2 \sum_{i<j} \nabla_i \nabla_j C = -2DC + 2 \sum_{i<j} \nabla_i \nabla_j C$$

and $\langle DC \rangle_0 = 0$ we have

$$\langle \gamma | \nabla^2 C | \gamma \rangle = 2 \sum_{i<j} \langle \nabla_i \nabla_j C \rangle_0. \quad (95)$$

Next observe $\partial_t C + \partial_x C + \partial_v C = -2(C^{(i,k)} + C^{(i,j)})$, where $C^{(i,k)}$ denotes the terms in $C$ that contain a $Z_j$ but not a $Z_k$, which gives

$$U_p^T X_k U_p = e^{i\gamma(C^{(i,k)} + C^{(i,j)})} X_k X_j.$$

Hence equation (62) follows by observing

$$\langle \nabla_i \nabla_j C \rangle_0 = \langle X_i X_j C - X_i C X_j - X_j C X_i + C X_i X_j \rangle_0$$

$$= (Ce^{-2\gamma(C^{(i,0)} + C^{(i,j)})} + e^{2\gamma(C^{(i,0)} + C^{(i,j)})} C)$$
$$= (Ce^{-2\gamma(C^{(i,0)} - C^{(i,j)})} + e^{2\gamma(C^{(i,0)} - C^{(i,j)})} C)$$
$$= 2(\sin(C^{(i,0)} + C^{(i,j)}) - 2\cos((\gamma C^{(i,0)} - C^{(i,j)}))C)$$
$$= -4(\sin(\gamma C^{(i,0)}) \sin(\gamma C^{(i,j)}))C_0$$
$$= -4(\sin(\frac{1}{2}\partial_t C + \frac{1}{2}\partial_x \partial_t C) \sin(\gamma \frac{1}{2}\partial_t C + \frac{1}{2}\partial_x \partial_t C))C_0$$

where we used $C^{(i,j)} = -\frac{1}{2}\partial_t C - \frac{1}{4}\partial_x \partial_t C$ and $\cos(a) - \cos(b) = -2\sin\frac{a+b}{2} \sin\frac{a-b}{2}$. \hfill \Box

**Proof of corollary 3.3.1.** Consider a general QAOA$_p$ state which we write shorthand as $|p\rangle := |\gamma \beta \rangle = \sum_q q_k \langle x | k \rangle$, where the coefficients $q_k \langle x | k \rangle$ may be complex. Proceeding as in the proof of theorem 3.3.1 gives to first order in $\beta$

$$\langle C \rangle_{p+1} \simeq \langle p | C | p \rangle + \beta \langle p \gamma_{p+1} | i \nabla C | p \gamma_{p+1} \rangle = \langle C \rangle_p + \beta \langle p | \nabla_B C | p \rangle$$

where $|p \gamma_{p+1} \rangle := e^{-i\gamma_{p+1} C} |p\rangle$ and $\tilde{B} = e^{i\gamma_p C} B e^{-i\gamma_p C}$. Observing that

$$\nabla_B C | p \rangle = -\sum_x \sum_i q_{x,i \neq p} \partial_c(x) e^{i\gamma_{p+1} \partial_c(x)} | x \rangle,$$

we have $\langle C \rangle_{p+1} \simeq \langle C \rangle_p - i\beta \sum_x q_{x,p} \left( \sum_{i=1}^n q_{x,i \neq p} \partial_c(x) e^{i\gamma_{p+1} \partial_c(x)} \right)$.

Next observe that

$$\sum_x \sum_{i=1}^n q_{x,i \neq p} q_{x,i \neq p} \partial_c(x) e^{i\gamma_{p+1} \partial_c(x)} \langle x | (x^{(j)}) - c(x) \rangle$$

$$= \sum_x \sum_{i=1}^n c(x) q_{x,i \neq p} q_{x,i \neq p} e^{-i\gamma_{p+1} \partial_c(x)} - q_{x,p} q_{x,i \neq p} e^{i\gamma_{p+1} \partial_c(x)}$$

$$= \sum_x \sum_{i=1}^n c(x) q_{x,i \neq p} q_{x,i \neq p} \left( e^{-i\alpha_{x,p}} - e^{i\alpha_{x,p}} \right) - q_{x,p} e^{i\gamma_{p+1} \partial_c(x)}$$

$$= \sum_x \sum_{i=1}^n c(x) r_{x,i \neq p} (2i \sin(\alpha_{x,p} + \gamma_{p+1} \partial_c(x)))$$

$$= -\sum_x \sum_{i=1}^n c(x) r_{x,i \neq p} \sin(\alpha_{x,p} + \gamma_{p+1} \partial_c(x))$$
where we have defined the real polar variables \(r, \alpha\) as \(q_{x,p} = |q_{e(p)}| p\), and \(q_{e(p)} = r_{x,p} e^{-i\alpha_{x,p}}\) which reflect the degree of which the coefficients \(q_{x,p}\) are non-real. Plugging in above implies \((84)\). Further, rearranging as
\[
\langle C \rangle_{p+1} \cong \sum_x c(x) \left( |q_{x,p}|^2 - 2\beta \sum_{j=1}^n r_{x,p} \sin(\alpha_{x,p} + \gamma_{p+1} \partial c(x)) \right)
\]
shows \((83)\) gives the change in probability for each state \(x\) to first order.

\[\square\]

### Appendix C. Norm and error bounds

Here we show bounds to the norms of cost gradient operators, which we subsequently apply to bound the error of our leading-order formulas.

The spectral norm \(\|A\| := \|A\|_2\) is the maximal eigenvalue in absolute value of \(A\). When \(C\) represents a function \(c(x) \geq 0\) to be maximized, for example a constraint satisfaction problem such as MaxCut or MaxSAT, then \(\|C\| = \max_x c(x)\). Hence computing \(\|C\|\) exactly can be NP-hard, in which case upper bounds to \(\|C\|\) (such as the number of clauses) typically suffice.

For commutator norms, commuting components should not affect the norm estimates, in particular the identity operator component of each operator. To reflect this in our norm and error estimates, here we define
\[
\|A\|_* := \min_{b \in C} \|A + bI\|,
\]
which in particular satisfies \(\|A\|_* \leq \|A\|\), and similarly for the traceless part of \(A\)
\[
\|A\|_* \leq \|A - \frac{1}{2} tr(A)I\|.
\]
As \(\|aI\|_* = 0\) for \(a \in C\), equation \((99)\) gives a seminorm.

For example, for MaxCut we have \(C = \frac{1}{2} I - \frac{1}{2} \sum \{j\} Z_j Z_j = \frac{1}{2} I + C_Z\) which satisfies \(\|C_Z\| = \|C\|_2\) and \(\|C\|_* = \sqrt{\frac{\|C\|}{2}}\). When \(c^* \neq |E|\) we have \(\|C\|_* < \|C - |E| I\|\) which illustrates that the inequality in equation \((100)\) can be strict.

#### C.1. Norm bounds

We first consider general gradients (commutators) \(\nabla G := [G, \cdot]\).

**Lemma C.1.1.** For \(n\)-qubit operators \(A, G\) and \(\ell \in \mathbb{N}\) we have
\[
\|\nabla^\ell G A\| \leq (2\|G\|_*)^\ell \|A\|_* \leq (2\|G\|_*)^\ell \|A\|.
\]
If we know a decomposition \(A = A_{com} + A_{nc}\) such that \([G, A_{com}] = 0\) then this improves to
\[
\|\nabla^\ell G A\| = \|\nabla^\ell G A_{nc}\| \leq (2\|G\|_*)^\ell \|A_{nc}\|_*.
\]

**Proof.** Let \(G' = G + gI\) and \(A' = A + aI\). As identity components always commute, trivially \(\nabla^\ell G A = \nabla^\ell G A\) for all \(g, a\). Selecting \(g, a\) such that \(\|G\|_* = \|G'\|^\ell\) and \(\|A\|_* = \|A'\|^\ell\) and applying the triangle and Cauchy-Schwarz inequalities to \(\nabla^\ell G A = G' A' - A' G'\) gives \(\|\nabla^\ell G A\| \leq \|G'\|^\ell \|A'\| \leq 2\|G'\|^\ell \|A'\| = 2\|G\|_* \|A\|_* \leq \|G\| \|A\|\). Equation \((101)\) then follows by induction on \(\nabla^\ell G A = \nabla^\ell G A_{nc}\). Equation \((102)\) follows by the same arguments observing \(\nabla^\ell G A = \nabla^\ell G A_{nc}\).

In particular, for the cost Hamiltonian \(C = a_0 I + C_Z\), lemma C.1.1 implies
\[
\|\nabla^\ell C A\| \leq (2\|C\|_*)^\ell \|A_{non-diag}\|.
\]
for \(A_{non-diag}\) the Pauli basis components of \(A\) that contain an \(X\) or \(Y\) factor.

For gradients \(\nabla^\ell\) with respect to the transverse-field Hamiltonian \(B\) we show a tighter bound applicable to \(k\)-local cost Hamiltonians. (Recall an operator is \(k\)-local if its Pauli expansion contains terms acting nontrivially on \(k\) or fewer qubits.)

**Lemma C.1.2.** For a \(k\)-local operator \(A\) and \(\ell \in \mathbb{N}\) we have
\[
\|\nabla^\ell A\| \leq (2k)^\ell \|A\|_* \leq (2k)^\ell \|A\|,
\]
and this bound is tight (i.e. there exists an \(A\) such that \(\|\nabla^\ell A\| = (2k)^\ell \|A\|_* = (2k)^\ell \|A\|\)).
Proof. Let $A' = aI + A$ such that $\|A\|_* = \|A\|$. In general $A' = \sum_j w_j \sigma^{(j)}$, where $w_j \in \mathbb{C}$ and each $\sigma^{(j)}$ gives a string of at most $k$ Pauli matrices. Consider the action of $\nabla = [B, \cdot] = \sum_i [X_i, \cdot]$ on a fixed $\sigma^{(j)}$; clearly, of the $n$ commutators $[X_i, \sigma^{(j)}]$ for $i = 1, \ldots, n$, at most $k$ can be nonzero. Moreover, each $[X_i, \cdot]$ either acts unitarily on a $\sigma^{(j)}$ (up to a factor of 2) if $\sigma^{(j)}$ contains a $Y_i$ or $Z_i$ factor, or else annihilates it. Hence $\|X_i, \sigma^{(j)}\| \leq 2\|\sigma^{(j)}\| = 2$ and so Cauchy-Schwarz gives

$$\|\nabla A\| = \|\nabla A'\| = \|\sum_j w_j [X_j, \sigma^{(j)}]\| \leq 2k\|A\|_* \leq 2k\|A\|.$$ 

Repeating this argument for $\|\nabla (\nabla^{\ell-1} A')\|$ gives the claim by induction.

Next, let $A = Z_1 Z_2 \ldots Z_k$ for some $k \leq n$; a straightforward calculation shows $\|\nabla^\ell A\| = (2k)^\ell \|A\|_* = (2k)^\ell \|A\| = (2k)^\ell$ for each $\ell = 1, 2, \ldots$ as desired.

Lemmas C.1.1 and C.1.2 may be applied recursively to bound $\|A\|$ for $A$ an arbitrary cost gradient operator as in lemma 2.4.1. Norm bounds are useful for upper bounding expectation values, as for any Hamiltonian $H$ and normalized quantum state $|\psi\rangle$ we have $\langle\psi|H|\psi\rangle \leq \|H\|$. For example, for MaxCut, lemma C.1.2 gives $(\langle(\nabla)^\ell C\rangle_p \leq 4\ell^2 \ell!$.

C.2. Error bounds

We now show how to obtain error bounds for commutator expansions, which we use to below to prove corollary 3.1.1 concerning the error of the estimates of theorem 2.2.1. The same approach may be applied to bounding the error when truncating our series expressions at higher order, or to deriving corresponding estimates for QAOA$_p$.

Here we utilize an integral representation of operator conjugation that follows from the fundamental theorem of calculus (see e.g. [64, equation 23])

$$e^{i\beta \nabla A} = A + i \int_0^\beta d\alpha e^{i\alpha \nabla} \nabla A,$$

which may be recursively applied to give

$$e^{i\beta \nabla A} = A + i \beta \nabla A - \int_0^\beta d\alpha \int_0^\alpha d\tau e^{i\tau \nabla} \nabla^2 A,$$ 

and similarly to pull out higher-order leading terms as desired.

Lemma C.2.1. For a $k$-local matrix $A$ acting on $n$ qubits we have

$$\|U_M^k(\beta) A U_M(\beta) - (A + i\beta \nabla A)\| \leq 2k^2 \beta^2 \|A\|_*.$$ 

Proof. Applying equation (106) with $U_M(\beta)$ and using Cauchy-Schwarz gives

$$\|U_M^k A U_M - A - i\beta \nabla A\| = \left\| \int_0^\beta d\alpha \int_0^\alpha d\tau e^{i\tau \nabla} \nabla^2 A \right\| \leq \left\| \int_0^\beta d\alpha \int_0^\alpha d\tau \| e^{i\tau \nabla} \nabla^2 A \| \right\| \leq \frac{\beta^2}{2} \| \nabla^2 A \| \leq 2k^2 \beta^2 \|A\|_* \leq 2k^2 \beta^2 \|A\|$$

where we have used $\|e^{i\tau \nabla} \nabla^2 A\| = \|\nabla^2 A\|$ from unitarity, and lemma C.1.2.

A similar argument yields an $O((2k|\beta|)^{\ell+1}\|A\|_*)$ error bound for truncating the series for $U_M^k A U_M$ at order $\ell$ (cf [64, theorem 5]).

Next bound the error of the quantities of theorem 2.2.1 as stated in corollary 3.1.1.

Lemma C.2.2. For QAOA$_1$ with $k$-local cost Hamiltonian $C$ the error in the estimate (13) of theorem 2.2.1 is bounded as

$$|\langle C \rangle_1 - (\langle C \rangle_0 - \gamma \beta (\nabla e \nabla C)_0) | \leq 4|\beta| \gamma^2 k \|C\|_*^2 + 4\beta^2 |\gamma| k^2 \|C\|_*^2.$$ 

Proof. Applying equations (105) and (106) to QAOA$_1$ we have
\[ e^{i \nabla C} e^{\beta \nabla^2 C} = C + i \beta e^{i \nabla C} - \int_0^\beta d\alpha \int_0^\alpha d\tau e^{i \nabla C} e^{\tau \nabla^2 C} \]
\[ = C + i \beta \nabla C - \gamma \beta \nabla C - \beta \int_0^\gamma d\alpha \int_0^\alpha d\tau e^{i \nabla C} e^{\tau \nabla^2 C} \]
\[ - \int_0^\beta d\alpha \int_0^\alpha d\tau \left( e^{i \nabla C} + i \int_0^\gamma d\epsilon e^{i \nabla C} e^{\epsilon \nabla^2 C} \right), \]

so taking the initial state expectation value of both sides and using \(|\nabla C|s\rangle = 0\) gives

\[ |\langle C \rangle_1 - \langle C \rangle_0 + \langle \nabla C \rangle_0| \leq |\beta| \int_0^\alpha d\alpha \int_0^\alpha d\tau e^{i \nabla C} e^{\alpha \nabla^2 C} \]
\[ + \beta \int_0^\alpha d\tau e^{i \nabla C} e^{\tau \nabla^2 C} \]
\[ \leq |\langle \nabla \rangle^2/2| \nabla C \nabla C \]
\[ \leq 4|\beta| |\gamma| \beta \gamma |\nabla C \nabla C|, \]

where we have used lemmas C.1.1 and C.1.2. Observing the left-hand side is invariant under shifts \(C \leftarrow C + a\) implies the tighter bound equation (107).

Naively apply the same approach to the error in the probability estimate of theorem 2.2.1 leads to a bound proportional to \(|\langle H \rangle|| \langle x | x \rangle|| = 1. Here we apply a refined analysis to obtain a more useful bound that reflects the exponentially small initial probabilities in the computational basis, at the expense of an exponential factor in the bound.

**Lemma C.2.3.** For QAOA, the error in the estimate (12) of theorem 2.2.1 satisfies

\[ |P_1(x) - P_0(x) - \frac{2 \beta \gamma}{2n} d(x)\rangle| \leq \frac{2}{2n} \left( n^2 \beta^2 e^{n|\beta|} + \frac{4}{3} n^2 |\beta| \gamma \beta |C| \cosh(2|\gamma| ||C||) \right), \]

(108)

**Proof.** Turning to the probability, for \(H_x = |x \rangle \langle x|\) we have

\[ e^{i \nabla C} e^{\beta \nabla^2 C} H_x = H_x + i \beta e^{i \nabla C} e^{\beta \nabla^2 C} + e^{i \nabla C} (- \frac{\beta^2}{2} \nabla^2 H_x - \frac{\beta^2}{3!} \nabla^3 H_x + \ldots) \]
\[ = H_x + i \beta \nabla H_x - \gamma \beta \nabla C + i \beta \left( - \frac{\gamma^2}{2} \nabla^2 H_x + \ldots \right) \]
\[ \left( \frac{\beta^2}{2} \nabla^2 H_x - \frac{\beta^2}{3!} \nabla^3 H_x + \ldots \right) \]

and so taking initial state expectations and using \(|\nabla H_x\rangle_0 = 0\) from lemma 2.5.2 gives

\[ P_1(x) - P_0(x) + \langle \nabla \nabla H_x \rangle_0 = \langle \gamma | R_1(\beta) | \gamma \rangle + i \beta | R_2(\gamma) \rangle_0 \]

for \(|\gamma \rangle := U_P(\gamma) |s\rangle\). For the first term on the right we have

\[ |\langle \gamma | R_1(\beta) \rangle | \leq \frac{1}{2^n} \sum_{|y|} e^{-\gamma (|x| - |y|)} |\gamma | R_1(\beta) | |y| \rangle \]
\[ \leq \frac{1}{2^n} \sum_{|y|} \sum_{|z|} |\gamma | R_1(\beta) | \langle y | z | \rangle \]
\[ \leq \frac{1}{2^n} \sum_{|y|} \sum_{|z|} |\gamma | \langle y | \nabla H_x | z \rangle | \]
\[ \leq \frac{1}{2^n} \sum_{\ell=1}^\infty \frac{|\beta| \ell}{\ell!} \sum_{|y|} \langle y | \nabla^\ell H_x | |z\rangle \]
\[ \leq \frac{2}{2^n} n^2 \beta^2 e^{n|\beta|} \]

where we have used \(\sum_{|y|} |\langle y | \nabla^\ell H_x | |z\rangle | \leq (2n)^\ell\), which follows observing that \(H_x\) has a single nonzero matrix element \(|x \rangle H_x | x \rangle = 1\) in the computational basis, and each application of \(\nabla\) increases the number of nonzero matrix elements (equal to \(\pm 1\)) by a factor at most \(2n\) (e.g. we have \(\nabla H_x = \sum_{j=1}^n |j \rangle \langle j | \nabla H_x | |j \rangle \langle j |\)).

Next, for the term corresponding to \(R_2(\gamma) = - \frac{\gamma^2}{2} \nabla^2 H_x - \frac{\gamma^3}{3!} \nabla^3 H_x + \ldots\), suppose we have shifted \(C\) such that \(|C||C| = ||C||_s\), which leaves \(R_2(\gamma)\) and other commutators invariant. Consider \(G := \nabla H_x\) which
similarly satisfies $\sum_{y,z}|\langle y|G|z\rangle| \leq 2n$. From lemma 2.5.1, when $\ell$ is even $\langle \nabla_\ell^\ell|G\rangle_0 = 0$, and for odd $\ell$ from expanding the commutators we have

$$\langle \nabla_\ell^\ell|G\rangle_0 = \frac{1}{2n} \sum_{y,z} |\langle y|\nabla_y^\ell|G|z\rangle| = \frac{1}{2n} \sum_{y,z} |\langle y|C^\ell G - \ell C^{\ell-1} GC + \cdots \pm GC^\ell|z\rangle|,$$

$$\leq \frac{2\ell}{2n} \|G\|e^\ell \sum_{y,z} |\langle y|G|z\rangle| \leq \frac{2\ell+1}{2n} \|G\|^\ell n,$$

which implies

$$\langle R_2(\gamma)\rangle_0 = | - i \frac{\gamma^3}{3!} \langle \nabla_0^3|\nabla_y^0 H_x\rangle_0 + i \frac{\gamma^5}{5!} \langle \nabla_2^5|\nabla_y^0 H_x\rangle_0 + \cdots |$$

$$\leq \frac{3n}{2} |\gamma|^3 \|G\|^3 \cosh(2\gamma \|G\|) \leq \frac{3n}{2} |\gamma|^3 \|G\|^3 e^{2\gamma \|G\|}.$$

Hence using $|P_1(x) - P_0(x) + \langle \nabla_y^0 H_x\rangle_0| \leq |\langle \gamma|R_1(\gamma)\rangle| + |\langle R_2(\gamma)\rangle_0|$ gives (108).

Finally, we use the lemmas to bound the error of the estimates of theorem 2.2.1.

**Proof of corollary 3.1.1.** From lemma C.2.2 for QAOA1 with $k$-local $C$ we have

$$|\langle C|_1 - (\langle C|_0 - \gamma \beta \langle \nabla_y^0 C\rangle_0)| \leq \|C\| \max(4|\beta| \gamma^2 k \|C\|^2 + 4\beta^2 |\gamma| k \|C\| \|C\|),$$

(109)

with $\langle \nabla_y^0 C\rangle_0 = 2 \langle CD| C\rangle_0$. Selecting $\gamma, \beta$ such that $|\beta| \leq \frac{\sqrt{\ell}}{2\ell}$ and $|\gamma| \leq \frac{e^{\ell/4}}{\ell \|C\|^2}$ gives

$$4|\beta| \gamma^2 k \|C\|^2 + 4\beta^2 |\gamma| k \|C\| \|C\| \leq \frac{\epsilon}{2} + \frac{\epsilon^{5/4}}{2} \leq \epsilon$$

which then implies equation (54) observing that $\|CZ\| \geq \|C\|$. Similarly, the probability bound follows from lemma C.2.3 applying the smaller mixing angle $|\beta| \leq \frac{\sqrt{\ell}}{2\ell}$ to equation (108) which gives an upper bound of $0.92\epsilon/2^n$ and implies equation (55).

**Appendix D. Quadratic Hamiltonians**

For $k$-local Hamiltonians, higher-order gradients have particularly nice properties\(^{19}\). Here we prove lemma 3.6.1 for QUBOs by considering the linear and quadratic terms in turn.

**Lemma D.0.1.** For a linear (1-local) cost Hamiltonian $C = \sum_q c_q Z_q$, we have

$$\nabla C = -2iC_Y \quad \text{and} \quad \nabla^2 C = 4C,$$

(110)

with $C_Y := \sum_q c_q Z_q$ which for $\ell \in \mathbb{N}$ implies

$$\nabla^{2\ell} C = 4^\ell C \quad \text{and} \quad \nabla^{2\ell+1} C = 4^\ell \nabla C.$$  

(111)

**Proof.** The lemma follows trivially from the Pauli matrix commutation relations as $\nabla Y = [X, C] = 2iC_Y$ and $\nabla^2 Y = 4c Z_Y$. The second statement follows by induction.

**Lemma D.0.2.** For a strictly quadratic (2-local) cost Hamiltonian $C = \sum_{uv} c_{uv} Z_u Z_v$, $C_Y = 0$, we have

$$\nabla^2 C = 8C - 8C_Y \quad \text{and} \quad \nabla^3 C = 16\nabla C,$$

(112)

with $C_Y := \sum_{uv} c_{uv} Y_u Y_v$, which for $\ell \in \mathbb{N}$ implies

$$\nabla^{2\ell} C = 16^{\ell-1} \nabla^2 C \quad \text{and} \quad \nabla^{2\ell+1} C = 16^\ell \nabla C.$$  

(113)

\(^{19}\) Recall an operator on qubits is (strictly) $k$-local if all terms in its Pauli operator expansion act nontrivially on at most $k$ qubits, and strictly $k$-local if all non-Identity terms act on exactly $k$ qubits.
Proof. The first statement follows trivially as before using the cyclic Pauli relations \([X_j, Y_j] = 2iZ_j\) and the linearity of \(\nabla = \{B, \cdot\}\), and the second by induction.

Lemma 3.6.1 then follows immediately from combining the linear and quadratic cases. Analogous results follow for \(k\)-local Hamiltonians with \(k > 2\).

D.1. QAOA\(_k\) for quadratic cost Hamiltonians

Lemma 3.6.1 may be applied directly to QAOA for QUBOs such as MaxCut where \(C = \frac{\theta}{4} - \frac{1}{2} \sum_{(ij) \in E} Z_iZ_j\). Recall the quantities of table 2.

Proof of equation (74). For MaxCut, applying lemma D.0.2 to (48) we have

\[
U_M^\dagger C U_M = \sum_{k=0}^{\infty} \frac{(i\beta)^k}{k!} \nabla^k C = C + \sum_{k=0}^{\infty} \frac{(i\beta)^k}{(2k)!} 16^k \nabla^2 C + \sum_{k=1}^{\infty} \frac{(i\beta)^k}{(2k)!} 16^{k-1} \nabla^2 C
\]

\[
= C + \frac{i}{4} \nabla C \sum_{k=0}^{\infty} \frac{(-1)^k (4\beta)^{2k+1}}{(2k+1)!} + \frac{1}{16} \nabla^2 C \sum_{k=1}^{\infty} \frac{(-1)^k (4\beta)^{2k}}{(2k)!}
\]

\[
= C + \frac{\sin(4\beta)}{4} i \nabla C + \frac{\cos(4\beta) - 1}{16} \nabla^2 C. \quad (114)
\]

Hence, using \(\cos(2x) = 1 - 2\sin^2(x)\), taking the expectation value with respect to \(|\gamma| := U_p(\gamma)|s\rangle\) gives equation (74) via \(\langle C \rangle = \langle |U_M^\dagger C U_M|\rangle = |\gamma|\langle |U_M^\dagger C U_M|\rangle\) and \(\langle C|C\rangle = \langle |s\rangle|s\rangle = \langle |\gamma\rangle|\rangle_0\).

The general QUBO formula (equation (77)) for \(\langle C \rangle\) is obtained similarly. Here we consider the explicit example of Balanced-Max-2-SAT as defined in section 3.6.1, which generalizes (and redefines along the way) previous results for QAOA\(_k\) for MaxCut. We emphasize the calculations such as that of the following proof for more general problems may be most easily implemented numerically, in particular for \(p > 1\) (cf. algorithm 2 in section 4.4).

Proof of equation (79) (and equations (75) and (76)). As \(C\) is strictly 2-local (modulo the identity term), equation (77) (cf equation (114)) gives \(\langle C \rangle = \langle |U_M^\dagger C U_M|\rangle\) with \(|\gamma| = U_p|s\rangle\) and

\[
U_M^\dagger C U_M = C + \frac{\sin 4\beta}{4} i \nabla C - \frac{\sin^2 2\beta}{8} \nabla^2 C. \quad (115)
\]

We follow but generalize the proof for MaxCut in [14, 17] (which is a simpler case with all signs the same of the ZZ terms in the cost Hamiltonian). Recall that in the Pauli basis only strictly \(I, X\) terms can contribute to QAOA initial state expectation values (i.e. if a Pauli string \(A_j\) contains a \(Y\) or \(Z\) factor then \(\langle s|A_j|s\rangle = Tr(|s\rangle\langle s|A_j\rangle) = 0\)). Observing that \(i\nabla C = -\frac{1}{2} \sum_{(ij) \in E} (-1)^{\delta_{ij}} (Y_iZ_j + Z_iY_j)\) (cf table 2) we have

\[
U_p^\dagger i \nabla C U_p = -\frac{1}{2} \sum_{(ij) \in E} (-1)^{\delta_{ij}} U_p^\dagger (Y_iZ_j + Z_iY_j) U_p
\]

\[
= -\frac{1}{2} \sum_{(ij) \in E} (-1)^{\delta_{ij}} (e^{2i\gamma C(|i\rangle\rangle_0} Y_iZ_j + e^{2i\gamma C(|j\rangle\rangle_0} Z_iY_j), \quad (115)
\]

where as the terms in \(C\) mutually commute we may write each exponential as a Pauli sum using \(e^{\pm i\gamma ZZ_{i}/2} = I \cos(\gamma/2) \pm i \sin(\gamma/2) Z_iZ_j\) and expanding the product. Clearly, the only resulting term that can contribute is proportional to \((-1)^{\delta_{ij}} Z_iZ_j \ast (-1)^{\delta_{ij}} Y_iZ_j = -iX_i\) (i.e. all other terms will contain at least one \(Z\) factor). Hence, as each \(C_{(i)}\) contains \(d_i + 1\) terms we have

\[
\langle |\gamma| i \nabla C |\gamma\rangle = \frac{1}{2} \sum_{(ij) \in E} \sin(\gamma/2)(\cos^d_i(\gamma/2) + \cos^d_j(\gamma/2)). \quad (116)
\]

(A nearly identical argument gives equation (75) for MaxCut after summing over the edges.)

Similarly, using \(\nabla^2 C = 8C - 8C_Y = -\frac{1}{4} \sum_{(ij) \in E} (-1)^{\delta_{ij}} (Z_iZ_j - Y_iY_j)\) gives

\[
U_p^\dagger \nabla^2 C U_p = 8C_Z + 2 \sum_{(ij) \in E} (-1)^{\delta_{ij}} e^{2i\gamma(C(|i\rangle\rangle_0 + C(|j\rangle\rangle_0)} Y_iY_j \quad (117)
\]

and so as \(\langle C_Z\rangle_0 = 0\) we have

\[
\langle |\gamma| \nabla^2 C |\gamma\rangle = 2 \sum_{(ij) \in E} (-1)^{\delta_{ij}} (e^{2i\gamma(C(|i\rangle\rangle_0 + C(|j\rangle\rangle_0)} Y_iY_j)_0. \quad (118)
\]
Consider a fixed edge \((ij)\) with \(d := \text{deg}(i) - 1\) and \(e := \text{deg}(j) - 1\) recall we define \(f^+ = f^+_0, f^- = f^-_0\) as the positive and negative triangles containing \((ij)\) the instance graph \(E\). For convenience here we let \(c = \cos(\gamma/2)\) and \(s = \sin(\gamma/2)\). Writing the exponential in equation (118) as a product of factors \(e^{i\gamma/2}Z_i Z_j / 2 = I_0 \pm isZZ\) and expanding gives a linear combination of \(2^{d+e}\) terms, which we view as a series in \(s\). The lowest order (w.r.t \(s\)) term that can contribute \[17\] corresponds to selecting a single triangle among the factors and is

\[
\left(\frac{f^+}{1}\right)^{d+e-2} - \left(\frac{f^-}{1}\right)^{d+e-2} = (f^+ - f^-)(f^+ - e^2)^{d+e-2},
\]

i.e. negative triangles subtract, and there are \(f^+, f^-\) ways to select a triangle of each type. (cf the corresponding proof for MaxCut where all triangles are positive \[14, 17\].) As \(f^+, f^-\) become larger, pairs of additional triangles can combine to \(\pm I\) such that the next contributing terms are proportional to \(e^{d+e-I}g\) and involve 3 triangles, with each sign determined by the number of positive- versus negative-parity triangles involved to give proportionality factor

\[
\left(\frac{f^+}{3}\right)\left(\frac{f^-}{0}\right) - \left(\frac{f^+}{0}\right)\left(\frac{f^-}{2}\right) + \ldots - \left(\frac{f^+}{0}\right)\left(\frac{f^-}{3}\right) + \ldots = \sum_{k=0}^{3} \left(\frac{f^+}{3-k}\right)\left(\frac{f^-}{k}\right)(-1)^k
\]

(i.e. three negative-parity triangles give \(-1\), and so on.)

Generalizing this argument to higher order, factors with \(\ell = 1, 3, 5\) triangles combine to contribute \(e^{d+e-2\ell}2^{2\ell}\) times the factor\[20\]

\[
\sum_{k=0}^{\ell} \left(\frac{f^+}{\ell-k}\right)\left(\frac{f^-}{k}\right)(-1)^k =: \left(\frac{f^+}{\ell}\right)_{2}F_{1}(-f^-, -\ell; f^+ - \ell + 1; -1)
\]

where \(2F_{1}\) is the Gaussian (ordinary) hypergeometric function \[77\]. Note equation (119) evaluates to \(f^+ - f^-\) for \(\ell = 1\), and to \(\left(\frac{f^+}{3}\right) - \left(\frac{f^-}{3}\right) - \frac{1}{2}f^+ f^- (f^+ - f^-)\) for \(\ell = 3\). Hence we have

\[
\langle e^{2\gamma(C(i)\X C(j)\Y)}Y_j Y_j \rangle_0 = e^{d+e-2}\sum_{\ell=1,3,5,\ldots} e^{2(f^+ - \ell)\ell/2} \left(\frac{f^-}{\ell}\right)_{2}F_{1}(-f^-, -\ell; f^+ - \ell + 1; -1)
\]

where we have defined \(g(f^+, f^-; \gamma, \beta) = \sum_{\ell=1,3,5,\ldots} e^{2(f^+ - \ell)\ell/2} \left(\frac{f^-}{\ell}\right)_{2}F_{1}(-f^-, -\ell; f^+ - \ell + 1; -1)\). It easy to see this term is 0 for all edges with \(f^+ = f^- \) or \(f = 0\), i.e. \(g(a, a) = 0\) for \(a = 0, 1, 2, \ldots\). Moreover, the case of strictly positive or strictly negative triangles \(g(f, 0) = -g(0, f)\) reproduces the analysis of MaxCut (up to constants) and is summable to give

\[
g(f, 0) = \frac{1}{2}(1 - (e^2 - s^2)f) = \frac{1}{2}(1 - \cos \gamma) = -g(0, f),
\]

which implies equation (76) for MaxCut.

Hence, we have \(\langle e^{2\gamma(C(i)\X C(j)\Y)}Y_j Y_j \rangle_0 = e^{d+e-2f^+ - 2f^-}g(f^+, f^-)\) and so \(\langle \gamma | \nabla^2 C | \gamma \rangle = 2\sum_{ij} e^{d+e-2f^+ - 2f^-}g(f^+, f^-)\), which together with the result for \(\langle \gamma | \nabla^2 C | \gamma \rangle\) gives equation (79).

\[\square\]

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\[20\] Without the factor \((-1)^k\) we would have Vandermonde’s identity \(\sum_{k=0}^{\ell} \left(\frac{f^+}{\ell-k}\right)\left(\frac{f^-}{k}\right)(-1)^k = \left(\frac{f^+}{\ell}\right)_{4}F_{4}(-f^-, -\ell; f^+ - \ell + 1; -1).\]
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