We adapt the Quantum Alternating Operator Ansatz (QAOA) to find ground states in quantum chemistry problems and empirically evaluate our protocol on several molecules. These simulations show robust qualitative behavior for QAOA as a function of the number of steps and size of the parameters. This includes cases where non-adiabatic schedules achieve state preparation accuracy close to that of the adiabatic limit while using relatively low quantum circuit depth. Simulations also show these behaviors in QAOA applied combinatorial search, providing evidence of the generality of these behaviors.

One of the most promising applications of quantum computing is simulating physical systems, for which a fundamental task is computing the energies of ground and excited states [1, 2]. Algorithms for this purpose include Hamiltonian simulation [3, 4] and quantum phase estimation [5], as well as variational approaches and related Lanczos type methods such as variational quantum phase estimation [6].

Many of these methods rely on being able to prepare a sufficiently good approximate ground or excited state. Adiabatic state preparation (ASP) [7–11] is one approach, which entails slowly evolving a known ground state of a simple system to the ground state of a system of interest. The system remains essentially in the ground state of the evolving Hamiltonian provided that the evolution time is large compared to the inverse square of the minimum gap between the first two energies [12]. In particular, this means the system will be in the target ground state at the end of the evolution.

A popular alternative to ASP, especially on near-term devices, is the variational quantum eigensolver (VQE) [13, 14]. This is an iterative process where, at each step, a sequence of parameterized quantum gates is applied to an initial state and the expected energy of the resulting state is measured. A classical algorithm uses the measurement results to adjust the gate parameters in an attempt to minimize the energy for the next measurement [13]. This quantum-classical hybrid method can work on NISQ devices [14], though finding good parameters can be prohibitively costly as the number of parameters increases with circuit depth [14–16].

In this paper we investigate a modified version of a distinct but related class of parameterized quantum circuits for finding molecular ground states and energies, the quantum approximate optimization algorithm (QAOA) [17–19] and its generalization to the quantum alternating operator ansatz [20] that incorporates broader classes of operators and states. QAOA has been demonstrated to outperform adiabatic techniques in certain contexts [21]. Research on QAOA has largely focused on combinatorial optimization problems encoded as a cost Hamiltonian $H_C$ whose ground state encodes the optimal problem solution. The level-$p$ QAOA algorithm uses $H_C$ and a “mixer” Hamiltonian $H_B$ as follows: An easy-to-prepare initial state, for example the ground
state of $H_B$, is prepared. For the originally proposed 
transverse-field mixer, the initial state is $|\psi_0\rangle = |+\rangle^\otimes N$, 
an equally weighted superposition over the computational 
basis. An alternating sequence of of length $2p$ of parameterized 
unitary operators is then applied to yield the state

$$|\psi_p(\tilde{\gamma}, \tilde{\beta})\rangle = e^{-i\tilde{\gamma}_p H_B} e^{-i\tilde{\gamma}_{p-1} H_C} \ldots e^{-i\tilde{\gamma}_1 H_B} e^{-i\gamma_0 H_C} |\psi_0\rangle.$$  

(1)

The state can then be measured to estimate quantities such as expectation values, and reprepared with updated 
parameters. For sufficiently large $p$ there exists a set of 
parameters that yields an arbitrarily good approximation 
to the ground state [17].

For applications in quantum chemistry, we evaluate 
QAOA performance in terms of the squared overlap of 
the final QAOA state with the ground state $|\phi_{gs}\rangle$:

$$\text{squared overlap} = \left|\langle \phi_{gs} | \psi_p(\tilde{\gamma}, \tilde{\beta}) \rangle\right|^2$$  

(2)

If there are degenerate ground states, this measure gener-
alizes to the sum of squared overlaps over all the ground 
states. As explained below, this performance metric is 
well-suited for applications such as chemistry, but gen-
erally less suitable for classical optimization, where the 
QAOA state may give good approximate solutions with 
little or no support on the true ground state.

There are a number of ways to select suitable param-
eters $\tilde{\gamma}, \tilde{\beta}$. One approach is optimizing all of the param-
eters. However, such optimization is expensive and may 
get stuck in local minima or encounter other bottlenecks 
such as exponentially small gradients [14]. Alternatively, one can define $\gamma_j$ and $\beta_j$ as functions of 
j specified by just a few parameters, thereby drastically 
reducing the number of free parameters to be optimized.

Through this research we study the regime of QAOA 
with $p \gg 1$ for which relatively few results exist in the 
literature. This enables identification of generic perform-
ance behavior expressed through what we term the 
QAOA phase diagram, which serves multiple purposes 
including a visualization of the performance of QAOA in 
the large $p$ limit. For the molecules that we consider, we 
empirically demonstrate that simple QAOA parameter 
schedules may offer significant improvement over algo-
rithms in the adiabatic regime.

**QAOA for chemistry:** We consider determin-
ing the ground state energy of a molecule with $n$ 
electrons, whose Hamiltonian is $H_e = \sum_{i<j} \eta_{ij} a_i^\dagger a_j + 
\sum_{ijkl} \eta_{ijkl} a_i^\dagger a_j^\dagger a_k a_l + \text{h.c.}$ where the $a_i$ ($a_i^\dagger$) are Fermionic 
annihilation (creation) operators in a molecular orbital 
basis, and h.c. denotes the Hermitian conjugate. In this 
second-quantized formulation the electronic Hamiltonian 
is quartic in the creation and annihilation operators for 
each orbital [22]. We also use the Hartree-Fock Hamilton-
ian, $H_{HF}$, which is diagonal in the basis of Slater 
determinants and defined by the energies of the single-
determinant Hartree-Fock approximate ground state and 
its excitations.

We truncate the Hilbert space and $H_e$ to $N > n$ single-
particle spin-orbitals, which account for both position 
and spin degrees of freedom. We consider the Jordan-
Wigner representation where Fermion occupation number 
bases are mapped to $N$-qubit computational basis 
states $|n_1 n_2 \ldots n_N\rangle$, which gives $H_e = \sum_{j=1}^m H_j = 
\sum_{j=1}^m c_j \sigma_j$, where $\sigma_j$ are strings of single-qubit Pauli 
operators. The number of terms is $m \sim N^4$, though this 
may be reduced substantially in particular basis set rep-
resentations.

a. **Differences from optimization setting** We present 
a modified version of QAOA adapted to chemistry appli-
cations. This requires a different strategy than for com-
binatorial optimization, where QAOA aims to find a low 
energy solution (bitstring) that is obtained by measuring 
the QAOA state. As quantum computers are not believed 
to be able to efficiently solve NP-hard problems, such 
approximate solutions are often the best we can hope to 
achieve, and the QAOA state may have little or no sup-
port on the ground states. This is a distinct goal from 
approximating the ground state in quantum chemistry, as 
generally the electronic Hamiltonian eigenstates are su-
perpositions of computational basis states, for which we 
are looking to generate a wave function whose squared 
overlap with the true ground state exceeds 99%. Hence 
in optimization, QAOA finds exact eigenvectors (approx-
imate solutions) and energies (cost function evaluations) 
and returns the best solution found, whereas in QAOA 
for chemistry we seek a state with high ground state over-
lap that is necessarily close in expected energy.

Chemistry applications differ from combinatorial opti-
mization in other regards. In particular, classical tech-
niques provide many useful starting approximations in 
quantum chemistry, which yields a well-motivated alter-
native to starting from an equal superposition of states 
in the Hilbert space [22]. In contrast, for optimization 
we often cannot do much better than random guessing in 
terms of initial state overlap with the optimal solution.

Chemistry has at least two simulation goals of interest: 
1) moderately accurate state preparation, that can be 
followed by further processing such as quantum phase 
estimation, and 2) state preparation that attains a high 
accuracy state for which the estimated energy will be 
chemically accurate. This study focuses on the second 
of these goals.

b. **QAOA Ansatz** Applying QAOA to chemistry re-
quires defining suitable cost and mixer Hamiltonians in 
Eq. 1 These must allow effective implementations, in-
cluding creating the initial state as the ground state of 
the mixer. We use the full Hamiltonian as the QAOA 
cost Hamiltonian, i.e., $H_C = H_e$.

Chemistry problems generally involve fixed particle 
number and fixed spin, and states that violate these 
quantities may be considered infeasible. Moreover, the 
Hartree-Fock state is an easily prepared feasible state [22] 
which typically has a relatively high squared overlap with 
the target state, i.e., the ground state of $H_e$. We take ad-
vantage of both these properties by using a mixer that re-
mains in the subspace of feasible states and whose ground state is the Hartree-Fock state. Specifically, we use the Hartree-Fock state as the QAOA initial state and the Hartree-Fock Hamiltonian as the mixer: $H_B = H_{HF}$. This mixer preserves state feasibility (i.e., cannot change particle number), and is relatively cheap to implement as $H_{HF}$ involves $\sim N^2$ operators, whereas $H_c$ generally requires $\sim N^4$ terms [22].

A notable consequence of this choice of mixer and cost Hamiltonians is that it inverts the properties of the standard QAOA setup: our cost Hamiltonian is non-diagonal in the computational basis while our mixer is diagonal. This choice is directly inspired by adiabatic state preparation, though our approach generalizes beyond the adiabatic regime, as discussed below. A similar QAOA construction is briefly mentioned in [21], although only in context of preserving symmetries.

In contrast to our choice of mixer, the standard transverse-field X mixer does not keep the state vector in the feasible subspace. In addition, as described in Appendix C while the XY mixer restricts evolution to the feasible subspace [20], the Hartree-Fock state is not its ground state. Thus these alternative mixers do not exploit the properties of the chemistry application as completely as the mixer we consider.

For simplicity and to reduce the dependence of our results on the quality of $\gamma, \beta$ found through classical optimization, we focus on QAOA parameter schedules defined by linear ramps

$$\gamma(f) = \Delta f \quad \text{and} \quad \beta(f) = \Delta (1 - f)$$

(3) where $\Delta$ is a constant and $f$ ranges from 0 to 1. The QAOA evaluation of Eq. 1 uses parameters sampled from these ramps: $\gamma_j = \gamma(f_j)$ and $\beta_j = \beta(f_j)$ where

$$f_j = \frac{j}{p + 1}$$

(4) with $j = 1, \ldots, p$. Similar linear schedules are frequently used for QAOA in optimization settings [18, 21, 25–28].

We investigate the efficiency of state preparation of various $\Delta$ and $p$ for several molecules. The product $\Delta p$ is roughly analogous to total annealing time of an analog version of this algorithm. We use the same $\Delta$ for both $\gamma_j$ and $\beta_j$ due to the commensurate energy scales of the cost and mixer Hamiltonians. These scales are similar because the mixer is the diagonal part of the cost Hamiltonian and the cost Hamiltonian is diagonal dominant for typical chemistry applications, and therefore determines the spectrum of the mixer.

c. QAOA phase diagrams To show QAOA performance we introduce QAOA phase diagrams. These diagrams show the squared overlap of Eq. 2 as a function of $\Delta$ and $p$. QAOA phase diagrams are a useful pictorial representation of how QAOA performs among different problems and parameter choices. Generalizing these diagrams to QAOA approaches that involve many variational parameters may not be as insightful.

Time dynamics algorithm: To test our approach on quantum chemistry applications and generate QAOA phase diagrams, we classically simulate systems of various sizes, including those that are generally larger than other studies with our recently introduced time evolution algorithm [11]. Doing a full configuration interaction (FCI) for the full cc-pVTZ orbital basis would require using up to $10^{19}$ determinants for the molecules we consider, which would be computationally infeasible. To circumvent this, we use a form of selective CI called adaptive sampling configuration interaction (ASCI) [29] to find the most important determinants for the first two eigenstates of our cost Hamiltonian, with the top $10^6$ determinants found for each. Due to the high squared overlap of our target state with our starting state, these determinants are the only ones necessary to capture the dynamics of our wavefunction as its squared overlap with the ground state changes with different parameter settings. The ASCI algorithm generates very accurate energies for electronic systems with strong many-body effects [29, 31] and provides an accurate description of time dynamics for wavefunctions close to the target ground state [11].

Molecular results: We tested our modified QAOA method on four molecules at their equilibrium geometries: P$_2$, CO$_2$, Cl$_2$, and CH$_2$. All these molecules have unique ground states, and were selected from the G1 set (55 molecules) [32]. Our choices are some of the harder molecules for our QAOA method because the squared overlap of their ground states with the Hartree-Fock state is lower than most molecules in this set. Specifically, the molecules we used have squared overlaps less than 0.9 [11, 23].

These test cases are somewhat large and would require over 100 logical qubits to test on quantum hardware. For P$_2$ ($N = 116$), Cl$_2$ ($N = 116$), and CH$_2$ ($N = 114$) the full cc-pVTZ orbital bases generated by Psi4 [33] were used, with only the first sixty-four spatial orbitals of the cc-pVTZ basis used for CO$_2$ ($N = 128$). The values of $\Delta$ explored ranged from 0.01 to 6, with values of $p$ from 1 to 100. For all cases considered in this work, the initial wavefunction is the ground state of the Hartree-Fock Hamiltonian so the behaviors seen in our studies approach the adiabatic limit in certain cases. For comparison, a recent study evaluating time evolution in the adiabatic limit with different schedules found that nearly linear interpolation between initial and target Hamiltonians outperformed all other monic polynomial interpolations [11].

Figure 1 shows the QAOA phase diagrams for our molecules. The white regions in these figures indicate parameter settings for which the squared overlap with the ground state decreases as a result of the protocol. We identify four main regions of interest in these diagrams:

a. Continuous adiabatic limit For very small $\Delta$ and very large $p$, QAOA becomes a close Trotter approximation to continuous evolution with a linear interpolation
In this case, the unitary QAOA operators for \( j \) correspond to the right edge of the phase diagrams. This roughly corresponds to the bottom right corner of the diagrams, a region where, in accord with the adiabatic theorem, the squared overlap with the target ground state goes to 1 as \( p \) increases. The corner itself is not completely yellow since the smallest values of \( \Delta \) we evaluated were so small that \( \Delta \) itself is not completely yellow since the smallest values of \( p \) target ground state goes to 1 as \( p \) increases. The corner corresponds to an improved squared overlap. White regions above the colored areas represent parameter settings where squared overlap with target ground state is less than its initial value.

of the mixer and cost Hamiltonians. In particular, when

\[
\Delta \to 0 \text{ and } \Delta p \to \infty
\]  

(5)

this approximation matches the adiabatic limit of continuous evolution. This roughly corresponds to the bottom right corner of the phase diagrams, a region where, in accord with the adiabatic theorem, the squared overlap with the target ground state goes to 1 as \( p \) increases. The corner itself is not completely yellow since the smallest values of \( \Delta \) we evaluated were so small that \( \Delta p \) is not large enough to approximate the limit of Eq. (5).  

b. Discrete adiabatic limit The other limit of particular interest is the discrete adiabatic limit \((\Delta > 0 \text{ is fixed and } p \to \infty)\) where

\[
\Delta > 0 \text{ is fixed and } p \to \infty
\]  

(6)

This corresponds to the right edge of the phase diagrams. In this case, the unitary QAOA operators for \( j = 1, \ldots, p \) change slowly as a function of \( j \), so the evolving state vector ends up almost completely overlapping with the target by the end (yellow edge) up to a particular \( \Delta \). For larger \( \Delta \), the overlap with the target ground state abruptly deteriorates (white edge). For these larger \( \Delta \), the state vector still evolves to an eigenstate of the cost Hamiltonian, but one that differs from the target.

c. Small \( \Delta \) The bottom half of each phase diagram shown in Figure 1 displays the expected monotonic improvement in QAOA performance with increasing \( p \) for small values of \( \Delta \). Moreover, in this region, for fixed \( p \), QAOA performance improves as \( \Delta \) increases, specifically for \( \Delta \) increasing over a range with length of about 0.3 to 0.7.

The regime of small \( \Delta \) and intermediate \( p \) corresponds to a situation where the discrete adiabatic limit closely follows the continuous due to Trotter approximation. Thus \( p\Delta \) increases as \( \Delta \) gets larger (for fixed \( p \)), corresponding to longer time for continuous adiabatic evolution. This, in turn, results in an improved overlap for fixed \( p \) and increasing \( \Delta \). In some cases, such behavior leads to choices of small \( \Delta \) with intermediate values of \( p \) giving even better overlaps than very small values of \( \Delta \) but large \( p \). At large, but fixed, \( p \), the limit \( \Delta \to 0 \)

FIG. 1. In order: (A) \( P_3 \) with initial squared overlap 0.77, (B) \( CO_2 \) with initial squared overlap 0.85, (C) \( Cl_2 \) with initial squared overlap 0.82, and (D) \( CH_2 \) with initial squared overlap 0.90. Colored regions are those where parameter settings result in an improved squared overlap. White regions above the colored areas represent parameter settings where squared overlap with target ground state is less than its initial value.

corresponds to a continuous evolution with a short time, which does not reach the adiabatic limit and gives worse performance than somewhat larger \( \Delta \) at that value of \( p \).  

d. Large \( \Delta \) For fixed \( p \), there is a sufficiently large value of \( \Delta \), which we denote \( \Delta_{\text{crit}}(p) \), above which QAOA performance starts to worsen, although not always monotonically. In particular, for the cases in Figure 1, \( \Delta_{\text{crit}}(p) \) is larger for small values of \( p \) than for large values of \( p \). Identifying, even roughly, the value of \( \Delta_{\text{crit}}(p) \) for intermediate \( p \) would allow maximizing the performance for such values of \( p \), thereby giving high overlaps with significantly fewer steps than required to get similar overlap from approaching the continuous adiabatic limit.

The qualitative behavior of QAOA shown in Fig. 1 is not specific to chemistry problems or our choice of mixer and initial state. This behavior also occurs for combinatorial optimization problems using the standard \( X \) mixer and uniform superposition initial state, as illustrated in Fig. 2 for a randomly generated instances of satisfiability (SAT) and the Ising model; see Appendix B for details.
The phase diagrams identify novel features of QAOA that have not been discussed in the literature. For example, in the parameter regime with large \( p \) and \( \Delta \) (upper right white regions in Fig. 1), the squared overlap tends toward zero as \( p \) increases. This behavior arises from a combination of the discrete adiabatic limit and how the QAOA operator eigenstates evolve during QAOA for different values of \( \Delta \) [34]. For large \( \Delta \), the eigenvalues of the unitary QAOA operator “wrap around” the unit circle of the complex plane, becoming indistinguishable from eigenvalues for a unitary matrix generated by a Hamiltonian with a different ordering of eigenvalues. Because of this, in the discrete adiabatic limit, following the instantaneous eigenvector of the QAOA operator that starts out close to the mixer Hamiltonian’s ground state does not result in reaching the cost Hamiltonian’s ground state by the end. Curiously, and very importantly, small scale model Hamiltonian simulations suggest following said eigenvector as \( p \to \infty \) still results in reaching a single eigenstate, rather than a superposition of such states. The eigenstate, however, is no longer the ground state of the cost Hamiltonian.

In some cases, as \( \Delta \) increases beyond \( \Delta_{\text{crit}}(p) \) the change in performance is not monotonic. For instance, the phase diagrams for phosphorus and chlorine (Figs. 1A and 1C, respectively) both have ridges with large squared overlap with the target extending to large \( p \) at \( \Delta \) somewhat larger than \( \Delta_{\text{crit}}(p) \).

**Conclusion:** This paper shows how to adapt QAOA to chemistry Hamiltonians, and illustrates its performance through QAOA phase diagrams. We used these diagrams to explore various QAOA parameter limits, including the continuous and discrete adiabatic regions. For the application to chemistry we demonstrated that non-adiabatic evolution can be more efficient than the adiabatic limit for the schedules considered in this work. A more detailed comparison of the methods would require finding optimal adiabatic and optimal QAOA schedules. In the context of optimization there is a close connection between optimal QAOA parameters and smooth adiabatic schedules [10, 28, 35, 36], showing conditions under which optimal schedules exist composed of “bang-bang” and “annealing” regimes, as well as the connection to counteradiabatic effects for suppressing excitations [37]. Cases where there are relatively few free parameters may be especially amenable to generalizations of our phase diagram approach. A future direction is to formally extend these results and other proposed approaches to analyzing QAOA (e.g., the perturbation series analysis of [38]), to the chemistry setting.

Through our analysis of QAOA phase diagrams and chemistry Hamiltonians, we found common qualitative features of near-adiabatic QAOA schedules, as illustrated in our figures, and why non-adiabatic schedules can show improvements. In particular, for the linear and nonlinear ramp schedules considered here, there is a region below a critical \( \Delta \) for which schedules lead QAOA to converge to the ground state. We demonstrate that for intermediate to small \( p \), away from the adiabatic limit, increased convergence to the ground state can still be attained. We show that these results extend beyond chemistry systems, including to combinatorial optimization, and so our phase diagrams help connect behaviors across multiple QAOA applications.

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Appendix A: Nonlinear Schedules

We use the linear ramps schedules defined in Eq. 3. However, nonlinear schedules can improve QAOA performance [21]. Additionally, nonlinear schedules improve the performance of adiabatic state preparation when they have slower changes in the neighborhood of small gaps [39]. To check the generality of the behavior seen in the QAOA phase diagrams (rather than improve the schedule, since nonlinear schedules haven’t shown much promise for molecular cases [11]), we examined two nonlinear ramps.

Since the minimum energy gap in our chemistry problems occurs at the end of the evolution [11], our first nonlinear schedule has smaller steps toward the end. We refer to this as the “root” schedule. Our second schedule, which we call the “tangent” schedule, takes larger steps at the beginning and end, and smaller steps in the middle. Our nonlinear schedules modify Eq. 3 by replacing $f$ at the beginning and end, and smaller steps in the middle, which we call the “tangent” schedule, takes larger steps

$F(f) = \sqrt{f}$

\[\text{(A1)}\]
and the tangent schedule is

\[
F(f) = \frac{1}{2 \tan(\frac{1}{2c})} \left( \tan\left( \frac{f - 0.5}{c} \right) + \tan\left( \frac{1}{2c} \right) \right) \tag{A2}
\]

where \( c = 0.37 \). Fig. 3 shows these choices of \( F(f) \) and contrasts them with the linear schedule.

For all four molecules, we find both nonlinear schedules produce the same qualitative features in the QAOA phase diagram as the linear schedule. Moreover, these nonlinear schedules do noticeably worse than the linear ramp, and do comparably as well as each other. The decrease in performance can be seen by the larger \( p \) required to reach over 0.99 squared overlap for small, non-zero \( \Delta \). To illustrate both of these points, Figs. 4 to 7 show the root and tangent ramps for the four molecules shown in Fig. 1.

FIG. 3. \( F(f) \) vs \( f \) for the nonlinear schedules

FIG. 4. Squared overlap with ground state after completing QAOA as a function of QAOA parameters \( \Delta \) and \( p \) for \( P_2 \), using (A) root, and (B) tangent schedules.

FIG. 5. Squared overlap with ground state after completing QAOA as a function of QAOA parameters \( \Delta \) and \( p \) for \( \text{CO}_2 \), using (A) root, and (B) tangent schedules.
Appendix B: Satisfiability and Ising spin problems

A SAT problem is to find an assignment, either true or false, to each of $n$ Boolean variables such that a given logical formula is true. For random 3-SAT, the formula is a conjunction of $m$ clauses. Each clause is a disjunction of a randomly selection of 3 distinct variables, each of which is negated with probability $1/2$. This instance has several ground states.

The Ising spin problem is to find the ground state of $n$ spins $s_i$, $i = 1, \ldots, n$ each of which is $\pm 1$. The fully-connected version illustrated here has Hamiltonian

$$H = \sum_i h_i s_i + \sum_{i<j} J_{i,j} s_i s_j$$

A random instance has the $h_i$ and $J_{i,j}$ selected independently and uniformly at random in the range $-1$ to $1$.

Appendix C: QAOA for Chemistry using XY-mixers

An alternative QAOA approach to chemistry and materials problems is using mixers related to the XY model, as previously proposed for graph coloring problems [20]. This mixer has the useful property of preserving total particle number, in contrast to the transverse-field mixer originally considered for QAOA. This alternative uses the same cost Hamiltonian as in the main text, i.e., $H_C = H_e$, but differs in the choice of initial state and mixing operator.

a. Initial states: Any linear combinations of strings with Hamming weight $n$ is feasible, corresponding to the $n$-electron sector of the Fock space. Following [20], we select such a feasible state as QAOA initial state. For example, we may again use the Hartree-Fock state. Alternatively, we could use the equal superposition of all $n$-particle basis states in $N$ orbitals, $\left(\begin{array}{c} N \\ n \end{array}\right)^{1/2} \sum_x |x\rangle$; such Dicke states can be constructed efficiently [40]. Note that here we relax the requirement that the initial state corresponds to the ground state of the mixing operator.

b. Mixing operator: By careful selection of the mixing Hamiltonian we can ensure the QAOA evolution remains in the feasible subspace [20]. In particular the Hamiltonian $H_B = \sum_{j<k} X_j X_k + Y_j Y_k$ which generates the XY mixer suffices; see [20 41] for other variants of this mixer with different resource tradeoffs. With this choice both the phase and mixing operators are nondiagonal in the computational basis. We emphasize that as the antisymmetry requirement of the problem is enforced by the state encoding (i.e., basis states correspond to Slater determinants), it is not necessary to select a mixer built from simple combinations of Fermionic operators.