Quantum optimization with Instantaneous Quantum Polynomial circuits

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We exploit the ability to embed 1-layer QAOA circuits into the larger class of parameterized IQP circuits to produce an improved variational quantum algorithm for solving combinatorial optimization problems. The 1-layer QAOA was recently shown to approximate low temperature pseudo-Boltzmann states, making it a suitable warm start for exploring the parameter space. We derive analytic expressions that allow us to explore the optimization landscape and find optimal parameters classically. The protocol is robust against barren plateaus and minimizes the necessary quantum resources compared to other traditional variational methods. We show numerically that the average overlap of the final state with the ground state scales like $\sim 2^{-0.31N}$ with the number of qubits $N$, a polynomial improvement over 1-layer QAOA, for random Sherrington-Kirkpatrick Hamiltonians of up to 29 qubits. Additionally, we show that performing variational imaginary time evolution on the manifold approximates low temperature pseudo-Boltzmann states, which may be used for sampling thermal distributions.

INTRODUCTION

Since its introduction by Farhi et al. \cite{Farhi2014} in 2014, the Quantum Approximate Optimization Algorithm (QAOA) has been explored in the quantum computing literature as one of the most promising heuristics for achieving quantum advantage on near-term devices \cite{Peruzzo2014, Kandala2017, Babbush2018}. This is only one example of a larger class of variational quantum optimization algorithms, which attempt to produce good solutions to combinatorial optimization problems by sampling a parameterized quantum circuit \cite{Montanaro2017, Romero2017, Bermejo2019, Chen2019, Babbush2019}. In the absence of quantum error correction protocols \cite{NC}, the required circuits must be sufficiently shallow to withstand noise, yet expressive enough to find states with high overlap onto the ground state. QAOA is a particularly good choice for satisfying these criteria, as it has an adjustable number of layers $p$. It can be understood as a Trotterized version of the quantum adiabatic algorithm (QAA), for which compelling theoretical evidence of performance exists \cite{Childs2009}. Additionally, it was shown that even for small numbers of layers, sampling from the QAOA ansatz is a hard task for classical computers \cite{Giovannetti2011}.

In this letter, we explore the embedding of the 1-layer QAOA into a broader class of variational circuits, the Instantaneous Quantum Polynomial (IQP) circuits, for which similar hardness of sampling theorems exist \cite{Gilyen2018}. These include a class of states called weighted graph states, which have been previously used in the tensor network community as a classical approach to solving quantum Hamiltonians \cite{Verstraete2004, Schuch2008}. The motivation is that the form of the Trotterized QAOA operators may not be the best choice at low depth. For this reason, instead of evolving the state according to the problem Hamiltonian, we give each parameter in the ansatz the freedom to evolve independently. By doing this, we find an ansatz of the same depth as 1-layer QAOA, but which may incorporate corrections that would otherwise require multiple layers.

Previous work on a similar approach claims that all local optima of the proposed ansatz \cite{Miciak2019} are eigenstates of the problem Hamiltonian. Such special cases of IQP circuits that produce computational states are not hard to sample, so do not provide a quantum advantage. We prove this statement is false by constructing a simple counterexample. This uncovers the possibility that sampling from some local minima of this ansatz need a quantum computer and may lead to an enhanced probability of finding the ground state. We give numerical evidence that such local optima exist in the vicinity of the optimal QAOA parameters, and have a high overlap onto the ground state. We note here that there may be other local minima of even lower average energy, but that does not guarantee their wavefunction has support on the problem solution. This makes starting the optimization from

FIG. 1. Diagrammatic representation of the algorithm. The 1-layer QAOA ansatz is a submanifold of the IQP ansatz and provides a warm start in the optimization protocol. The trajectory between the QAOA optimum and the IQP optimum is defined via the McLachlan variational principle and is computed classically. Colour coding the optimization landscape represents the effective temperature of the associated state, with lower temperature states (blue) having a higher chance of sampling the ground state. The quantum computer is only used during the sampling step, which is known to be difficult classically.
QAOA an essential step of the algorithm. We derive efficient analytic and exact expressions for the cost function and its gradients, which allow us to train the model classically and bypass typical limitations such as the appearance of barren plateaus [17]. Since the depth of our circuits increases linearly with the number of qubits, this result is independent and expands upon light cone based methods [15]. This leaves only the key ingredient of sampling from the final quantum state to be performed on the quantum device, as illustrated in Fig. 2.

The vicinity of the optimal QAOA location on the manifold is also interesting from a different perspective. A recent investigation of the states produced by 1-layer QAOA [19] shows that sampling produces a distribution close to a Boltzmann distribution, at temperatures beyond the reach of classical sampling techniques such as Markov Chain Monte Carlo (MCMC) [20]. We improve on this result by lowering the temperature further, using variational quantum imaginary time evolution (VQITE) [21]. However, the constraint of having the state remain on the variational manifold limits our ability to follow exact imaginary time evolution and distorts the distribution. We only take a small number of steps in order to mitigate this effect.

The structure of our algorithm can be natively described in terms of all-to-all two-qubit interactions with adjustable phase, making its implementation most natural for ion trap quantum computers. This makes it a great candidate for showing a quantum advantage in solving optimization problems in the near future.

**THE QUANTUM APPROXIMATE OPTIMIZATION ALGORITHM**

The standard implementation of the QAOA [1] attempts to create states with large overlap onto the ground eigenspace of some optimization problem, typically defined through an Ising Hamiltonian,

$$H = \sum_{i} h_i Z_i + \sum_{(i,j)} J_{ij} Z_i Z_j, \quad (1)$$

where the $Z_i$ variables can be interpreted as the projections onto the Z axis of a classical or quantum mechanical ensemble of $N$ spin-$\frac{1}{2}$ particles and $(h_i, J_{ij})$ are real coefficients. This is achieved by starting with the ground state $|+\rangle^\otimes N$ of the trivial transverse field mixing Hamiltonian $H_x = \sum_i X_i$ and evolving it under the alternating application of the propagators of $H$ and $H_x$. The final trial state is of the form

$$|\Psi(\gamma, \beta)\rangle = \prod_{k=1}^{p} \exp(-i\beta_k H_x) \exp(-i\gamma_k H) |+\rangle^\otimes N, \quad (2)$$

where $p$ is called the level of the QAOA and the real coefficients $\beta_k$, $\gamma_k$ are used as variational parameters. The most commonly used cost function in the optimization of the ansatz is the expectation value of the problem Hamiltonian

$$E = \langle \Psi(\gamma, \beta) | H | \Psi(\gamma, \beta) \rangle, \quad (3)$$

although alternative objective functions have been proposed [22, 23]. Since the QAOA may be thought of as a discretized version of QAA, we expect the global minimum of this variational manifold to have a large overlap with the solution of the problem. For the rest of this work, we will only consider the 1-layer QAOA, which is sufficiently shallow to withstand the effects of noise and obtains a good ground state overlap [19].

**THE INSTANTANEOUS QUANTUM POLYNOMIAL CIRCUIT**

The IQP is a non-universal model of quantum computation with similar roots to the boson sampling problem, whose aim is to strengthen the general belief that quantum computers are more powerful than classical machines [24]. In order to define the IQP, let $N = \{1, 2, \ldots, N\}$ be a set of qubit labels and denote by $2^N$ the powerset (set of all subsets) of $N$. We now define the IQP Hamiltonian as the sum over a mutually commuting set of Pauli operators given by $H_{\text{IQP}}(\vec{\theta}) = \frac{1}{2} \sum_{e \subseteq 2^N} \theta_e Z_e$, where $Z_e = \bigotimes_{i \in e} Z_i$ is the Z operator with support on subset $e$ and $\theta_e$ are real coefficients. Throughout the work we will only make use of IQPs with single and two-body operators, which we refer to as an SD-IQP. This means, for an SD-IQP, the sum only includes terms with support $|e| \leq 2$. For this class, we employ the simplified notation $H_{\text{IQP}}(\vec{\theta}) = \frac{1}{2} \sum_{e \subseteq 2^N} \theta_e Z_e + \frac{1}{2} \sum_{i,j} \theta_{ij} Z_i Z_j$. The IQP problem is then to sample the probability distribution given by measuring the state

$$|\Psi_{\text{IQP}}\rangle = H^\otimes N \exp\left(-iH_{\text{IQP}}(\vec{\theta})\right) |+\rangle^\otimes N, \quad (4)$$

in the computational basis of all qubits, where $H$ is the Hadamard gate. In [12], it is shown that this is a hard task for a classical computer under certain widely believed complexity theoretic assumptions. Here, we make the important observation that, up to single qubit rotations and energy rescaling, the IQP state in Eq. (4) is the same as that produced by a 1-layer QAOA designed to solve for the ground state of $H_{\text{IQP}}$. To make this connection more precise, consider the following variational ansatz

$$|\Psi(\vec{\theta})\rangle = \bigotimes_{i \in N} R_x(\phi_i) \cdot \exp\left(-iH_{\text{IQP}}(\vec{\theta})\right) |+\rangle^\otimes N, \quad (5)$$

where $R_x(\phi) = \exp(-i\phi X/2)$ and $\vec{\theta} = (\vec{\phi}, \vec{\theta})$ are free, real parameters. This generalizes the optimization cost of Eq. (3) function to
FIG. 2. Optimization results for 300 randomly generated Sherrington-Kirkpatrick Hamiltonians of up to 29 spins. a) Probability of sampling the ground state configuration in the optimal IQP ansatz. b) Enhancement factor $p_{\text{IQP}}/p_{\text{QAOA}}$ for finding the ground state in the optimized IQP ansatz compared to the original QAOA. Using a linear fit we find the average probability of sampling the ground state $p_{\text{IQP}} \sim 2^{-\alpha N}$ with $\alpha = 0.31 \pm 0.02$ and the average enhancement factor $p_{\text{IQP}}/p_{\text{QAOA}} \sim 2^{\delta N}$ with $\delta = 0.23 \pm 0.02$. The errors indicate the variability in gradient at one standard deviation, also shown in the plots. The statistics are performed using the logarithms of probabilities.

$$E(\theta) = \langle \Psi(\theta) | H | \Psi(\theta) \rangle = \langle \mathcal{H} \rangle_\theta, \quad (6)$$

which we refer to as the optimization landscape.

Since the IQP state defined in Eq. (4) can be brought to this form by a final layer of single qubit rotations, we also expect generic states of this form to be difficult to sample classically. The task of computing the cost function defined in Eq. (6) is then reduced to estimating the expectation values of the spins $(Z_i)\theta$ and correlators $(Z_iZ_j)\theta$ in an arbitrary state $|\Psi(\theta)\rangle$. The mixing layer rotates the middle $Z$ operators into products that contain $X$ operators, which then anticommute with some terms in $H_{\text{IQP}}$. In Appendix A, we show that the latter expression can be reduced to calculating partition functions of reduced Ising Hamiltonians of the form

$$Z_e = \frac{1}{2^N} \sum_{\{x\}} e^{-iH_e(x)}, \quad (7)$$

where $e$’s are single or two qubit subsets of $\mathcal{N}$. The reduced generator $H_e$ retains only the terms in $H_{\text{IQP}}$ that anti-commute with the operator $X_e = \bigotimes_{i \in e} X_i$. This leads to a highly restricted graph topology, for which partition functions can be evaluated exactly. We generalize this method to show that SD-IQPs have simple analytic expressions for all expectation values of the form $(Z_e)\theta$, with a number of terms that scales like $O(2^{|e|})$. This result generalizes previous analytical expressions used in QAOA calculations to the case of all-to-all connectivity problems with arbitrary weights [25,27]. These properties of the SD-IQP ansatz make it an excellent candidate for solving optimization problems, as it is guaranteed to be at least as powerful as 1-layer QAOA and the training can be performed efficiently using only classical resources. The access to exact, analytic expressions for the cost function also means we do not need to worry about barren plateaus, finite sampling or device errors during training. Access to a quantum computer is only necessary during the final sampling step, so we expect our protocol to perform well on NISQ devices.

As opposed to the standard QAOA ansatz, the SD-IQP is sufficiently flexible to produce all computational states. In particular, this means that, if a classical algorithm were able to find the global optimum of Eq. (6), it would also find the exact ground state of $H$. In [16], it is shown that the optimization landscapes of IQP ansatze with only polynomially many terms are generally non-convex and computational states other than the solution may form local minima, which we call trivial minima. Consequently, converging to such local minima would imply the algorithm does not need access to a quantum computer, as the bits $x_i$ of the solution corresponding to the optimal parameters are given by $(Z_i)\theta$, which can be efficiently computed classically.

Despite these drawbacks, we prove that the optimization landscapes can contain non-trivial minima, and give a minimal example of this in Appendix D. Remarkably, we provide numerical evidence that such a local minimum is located in the vicinity of the QAOA parameters, and show that sampling the IQP circuit at this point greatly enhances the chance of finding the ground state compared to QAOA.
McLachlan variational principle [21, 29] parameters in the ansatz are evolved according to this operator leads to a decrease in temperature. The initial state is pseudo-Boltzmann as in Eq. 8 applying \( e^{-\beta H} |+\rangle \otimes N \), with large inverse temperature \( \beta \), up to relative phases that do not affect the distribution. This is important because sampling this state produces the same distribution as sampling the mixed thermal state \( \rho_\beta = e^{-\beta H} / Z \) for classical Hamiltonians, which is useful for a variety of optimization tasks. In our work, we use this result to justify the 1-layer QAOA as a good starting point in optimizing the SD-IQP ansatz. Since the 1-layer QAOA ansatz can be recovered by restricting the parameters of the full SD-IQP, we find the optimal QAOA position classically, using the Broyden–Fletcher–Goldfarb–Shanno (BFGS) [28] algorithm on the submanifold. To find a local optimum in the vicinity of this position, it is sufficient to use simple gradient descent. However, we are also interested in producing low temperature states, which is achieved using a different approach called VarQITE. This protocol aims to find the trajectory on the manifold that best approximates the action of \( \exp\{-\tau H\} \) on the state. If the initial state is pseudo-Boltzmann as in Eq. 8 applying this operator leads to a decrease in temperature. The parameters in the ansatz are evolved according to the McLachlan variational principle [21, 29]

\[
A \frac{d}{d\tau} \theta = -\frac{1}{2} \nabla E(\theta),
\]

where the coupling matrix \( A \) describes the geometry of the variational manifold (i.e. it is the Gram matrix of the tangent vectors corresponding to each parameter) and \( \tau \) is the imaginary time variable. In Appendix B we show that the coefficients of the Gram matrix can be expressed as expectation values of low-weight Pauli operators in the IQP, for which we find simple analytic expressions. This linear system of ODE’s defines a flow on the variational manifold, that we solve numerically using the Runge-Kutta method [30]. We stop this procedure when we arrive at a local minimum, or when \( A \) becomes non-invertible. This typically happens after a long plateau in the energy profile, which we illustrate in Appendix C. This becomes a rare occurrence when we increase the number of qubits, but for problems that exhibit this behaviour we choose the optimal parameters in the middle of the plateau. After finding the optimal parameters, we use Qiskit quantum simulators [31] to sample the circuit and compute the probability of finding the ground state. We share the code used for implementing this protocol in [32].

Additionally, we would also like to assess the quality of our thermal states. To do this, we introduce the Kullback-Leibler divergence (KL), defined as

\[
D_{KL}(P \parallel Q_\beta) = \sum_x P(x) \log \frac{P(x)}{Q_\beta(x)},
\]

where \( x \) runs over all bitstrings of length \( N \), \( P(x) \) is the distribution produced by our IQP circuit and \( Q_\beta(x) \) is a model distribution, which we choose to be the thermal distribution at some inverse temperature \( \beta \). By optimising over \( \beta \), we find the thermal distribution which best approximates the output of our IQP. For characterization purposes, we do this by computing the KL divergence exactly, but in practice this would be estimated from samples [33].

RESULTS

We test our method on Sherrington-Kirkpatrick Hamiltonians [34, 35] of up to \( N = 29 \) spins, which are of the form of Eq. (1) with \( h_i = 0 \) and \( J_{ij} \) independent and identically distributed Gaussian random variables of 0 mean and a standard deviation of \( 1 / \sqrt{N} \). This Hamiltonian has a \( \mathbb{Z}_2 \) symmetry, so the ground state is unique up to flipping all qubits. In Fig. 2 we show how the overlap of the optimized IQP state onto the ground eigenspace varies with the problem size, as well as how it compares to the initial QAOA. Both plots show a clear exponential trend with relatively low and slowly increasing variance. This confirms that our algorithm has a significantly better exponential scaling compared to 1-layer QAOA. We note that it tends to perform better and have fewer outliers as we increase the number of qubits. We also study how the temperature of the distribution changes as we perform imaginary time evolution on our variational manifold up to time \( \tau = 10 \), close to
convergence. In Fig. 3 we show how the optimal normalized temperatures differ in the starting QAOA state and the final optimized IQP state. The KL divergence from the optimized IQP state to the best fitting thermal state is higher, but it appears to stagnate compared to the linearly increasing divergence observed in the QAOA states. This may indicate that this discrepancy between the IQP and the QAOA vanishes, or even flips, as we increase the problem size. In Fig. 4 we plot example distributions produced by the QAOA and optimized IQP ansatze. From the qualitative aspect of the IQP distribution, we see that the performance of our algorithm in increasing the ground state overlap cannot be entirely explained as a consequence of having a lower temperature. The distribution becomes arched, and the probabilities of sampling the low energy eigenstates rise orders of magnitude above the predictions of the thermal fit. Future theoretical work is necessary to understand how this effect emerges, and whether it is recovered in more general optimization problems.

DISCUSSION

The algorithm we introduce explores the natural connection between the 1-layer QAOA state and the IQP circuits, both of which have been proven difficult to sample classically. Studying the position of the QAOA in this broader variational manifold leads to a better understanding of its optimality as a shallow depth quantum heuristic, as well as how it can be improved.

We show that, for the case of fully connected Sherrington-Kirkpatrick Hamiltonians, our approach produces a large amplification of the probability of sampling the ground state, beyond what can be obtained using classical tools such as MCMC. Since the improvement over simple unstructured search is better than quadratic, it may compensate the slowdown from quantum error correction when applied to large problems [36]. The hardware implementation is identical, and parameter training can be performed classically in time $O(N^3)$, making it a strong candidate for showing a quantum advantage on near-term devices. Since the ansatz is expanded to an all-to-all connectivity, we also expect to bypass many of the limitations of QAOA that rest on locality [37] or symmetry [38, 39].

This amplification asks for a better theoretical understanding of shallow QAOA circuits, where the errors introduced by discretizing QAA are important. Generalizing our approach to multi-layered QAOA is straightforward, but whether analytic trainability is possible in this case is an open question. Even if the gradients of the cost function are evaluated from samples, providing the algorithm with a warm start, i.e. the QAOA optimal parameters, may be sufficient to overcome typical limitations such as the barren plateaus [40, 41].

Another possible route to improve our results is to add extra terms in the IQP ansatz, such as three-body terms $Z_i Z_j Z_k$. These extra terms may be particularly important in the context of constrained optimization problems, as they may allow direct transitions between bit-strings with larger Hamming distance that satisfy the constraints. If we use the same method as for the SD-IQP to express the expectation value of the Hamiltonian as a sum of partition functions as in Eq. (7), the three body operators will become two body terms in the partition function. This means that analytically computing the expectation value of a Hamiltonian in the IQP that also includes all three body terms is reduced to computing the partition function of arbitrary graphs, which is
hard in general. It is then important to select which terms to include so the optimization remains tractable.

If the problem Hamiltonian does not have all-to-all connectivity, the IQP demands more operations on the quantum device than 1-layer QAOA, making the comparison unfair. Therefore, we restricted the analysis to Sherrington-Kirkpatrick Hamiltonians. It would be interesting to study if similar performance is obtained for different problems, such as MaxCut. In these cases, the problem Hamiltonian may not include all two-body operators, so promoting the QAOA to an IQP ansatz will introduce additional gates into the circuit. We would also like to understand how our algorithm performs for large problems, where finding the exact ground state is unlikely. We leave it as future work to characterize the approximation ratio we can achieve for different realistic problems, and compare with the best known classical methods.

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Appendix A: Analytic expression for expectation values in the IQP state

In this appendix we show how to derive exact analytic expressions of expectation values of low-weight Pauli operators in the SD-IQP ansatz. Let $P_e$ be some Pauli string that applies non-identity Pauli operators to a subset of qubits $e \in \mathcal{N}$ and let $w_e = |e|$ be the weight of $P_e$. If we identify Pauli strings that differ only by a phase, we can characterize them using two length-$N$ boolean vectors $a, b \in \mathbb{Z}_2^N$ by the decomposition $P_e = Z^a X^b$, where we used the notation $Z^a = \bigotimes_{i=1}^N Z^{a_i}$. Denote by $e_Z$ and $e_X$ the subsets of $\mathcal{N}$ corresponding to the nonzero elements of $a$ and $b$ respectively, and let $w_a = |e_Z|$ and $w_b = |e_X|$ be corresponding weights. Our goal is then to compute $\langle Z^a X^b \rangle_\theta$. First, we show how the layer of single qubit $X$ rotations transforms this operator

$$\prod_{i \in \mathcal{N}} R^x_i(\phi_i) Z^a X^b \prod_{i \in \mathcal{N}} R^x_i(\phi_i) = \prod_{i \in \mathcal{N}} (R^x_i(\phi_i) Z R^x_i(\phi_i))^{a_i} (R^x_i(\phi_i) X R^x_i(\phi_i))^{b_i} = \prod_{i \in \mathcal{N}} (\cos \phi_i Z + \sin \phi_i Y)^{a_i} X^{b_i}. \quad (A1)$$

This can be expanded to a sum of $2^{w_a}$ Pauli strings, whose expectation values are then to be calculated in the state $\exp(-iH_{\text{IQP}}) \ket{+}^\otimes N$. To simplify notation we will denote all expectation values in this state by $\langle \cdot \rangle$, which differs from the expectation value in the full ansatz by omitting the subscript $\theta$. If we recycle previous notation for brevity, we are now interested in computing expectation values of the form

$$\langle Z^a X^b \rangle = \langle + \rangle^\otimes N \exp(iH_{\text{IQP}}) Z^a X^b \exp(-iH_{\text{IQP}}) \ket{+}^\otimes N. \quad (A2)$$

Since we are only working with SD-IQPs we can expand the Hamiltonian as

$$H_{\text{IQP}} = \frac{1}{2} \sum_{i \in \mathcal{N}} \theta_i Z_i + \frac{1}{2} \sum_{\{i,j\}} \theta_{ij} Z_i Z_j. \quad (A3)$$

The terms in the Hamiltonian that commute with $Z^a X^b$ can be straight-forwardly cancelled out, while those that anti-commute with $Z^a X^b$ can be moved through with a flipped sign. Then we have

$$\langle Z^a X^b \rangle = \langle + \rangle^\otimes N \sum_{\{x\}} Z^a \exp(i \sum_{i \in e_X} \theta_i Z_i + i \sum_{i \in e_X, j \notin e_X} \theta_{ij} Z_i Z_j) X^b \ket{+}^\otimes N$$

$$= \frac{1}{2^N} \sum_{\{x\}} \langle x \rangle Z^a \exp(i \sum_{i \in e_X} \theta_i Z_i + i \sum_{i \in e_X, j \notin e_X} \theta_{ij} Z_i Z_j) \ket{x}, \quad (A4)$$

where in the last equality we expanded the state $\ket{+}^\otimes N$ as a sum over all spin configurations $x_i \in \{+1, -1\}$ and made use of the fact that the central operator is manifestly diagonal in this basis. We can absorb the $Z^a$ in the propagator by noting that $\exp(-i\pi Z/2) = -iZ$ and using the transformed angles $\tilde{\theta}_i = \theta_i - a_i \pi/2$, giving us the simple expression

$$\langle Z^a X^b \rangle = \frac{i^{w_a}}{2^N} \sum_{\{x\}} \exp(i \sum_{i \in e_X} \tilde{\theta}_i x_i + i \sum_{j \notin e_X} x_j \left(-\frac{\pi}{2} a_j + \sum_{i \in e_X} \theta_{ij} x_i\right)). \quad (A5)$$

This form has the interpretation of a partition function over the bipartite graph formed by splitting the set of all qubits $\mathcal{N}$ into $e_X$ and its complement. This suggests we should separate the spins corresponding to different subsets, so we will denote by $r$ the configurations of spins in $e_X$ and by $s$ configurations of the complement. The expression is then rewritten as
\[
(Z^a X^b) = \frac{i^{w_a}}{2^N} \sum_{\{s,r\}} \exp \left( i \sum_{i \in e_X} \theta_i r_i + i \sum_{j \notin e_X} s_j \left(-\frac{\pi}{2} a_j + \sum_{i \in e_X} \theta_{ij} r_i \right) \right)
\]
\[
= \frac{i^{w_a}}{2^N} \sum_{\{r\}} \exp \left( i \sum_{i \in e_X} \theta_i r_i \right) \prod_{j \notin e_X} \left(\sum_{y \in \{+1,-1\}} (-iy)^{a_j} \exp \left( i \sum_{i \in e_X} \theta_{ij} r_i y \right) \right)
\]
\[
= \frac{i^{w_a}}{2^N} \sum_{\{r\}} \exp \left( i \sum_{i \in e_X} \theta_i r_i \right) \prod_{j \notin e_X} Q_{a_j} \left(\sum_{i \in e_X} \theta_{ij} r_i \right)
\]

which is now a sum over the configurations of spins in \(e_X\) only. For simplified notation we introduced the \(Q\) function, which is defined as

\[
Q_0(x) = \cos x,
\]
\[
Q_1(x) = \sin x
\]

We can simplify this even further by grouping configurations that differ only by the \(\mathbb{Z}_2\) operation of flipping the sign of all spins to obtain

\[
\langle Z^a X^b \rangle = \frac{i^{w_a}}{2^w_b} \sum_{\{r\}/\mathbb{Z}_2} \left[ \exp \left( i \sum_{i \in e_X} \theta_i r_i \right) \prod_{j \notin e_X} Q_{a_j} \left(\sum_{i \in e_X} \theta_{ij} r_i \right) + \exp \left( -i \sum_{i \in e_X} \theta_i r_i \right) \prod_{j \notin e_X} Q_{a_j} \left(-\sum_{i \in e_X} \theta_{ij} r_i \right) \right]
\]
\[
= \frac{i^{w_a}}{2^w_b} \sum_{\{r\}/\mathbb{Z}_2} \left[ \exp \left( i \sum_{i \in e_X} \theta_i r_i \right) \prod_{j \notin e_X} Q_{a_j} \left(\sum_{i \in e_X} \theta_{ij} r_i \right) + \exp \left( -i \sum_{i \in e_X} \theta_i r_i \right) \prod_{j \notin e_X} Q_{a_j} \left(-\sum_{i \in e_X} \theta_{ij} r_i \right) \right]
\]
\[
= \frac{i^{w_a}}{2^w_b} \sum_{\{r\}/\mathbb{Z}_2} \left[ \exp \left( i \sum_{i \in e_X} \theta_i r_i \right) \prod_{j \notin e_X} Q_{a_j} \left(\sum_{i \in e_X} \theta_{ij} r_i \right) + (-1)^{a_P} \exp \left( -i \sum_{i \in e_X} \theta_i r_i \right) \prod_{j \notin e_X} Q_{a_j} \left(-\sum_{i \in e_X} \theta_{ij} r_i \right) \right]
\]
\[
= \frac{i^{w_a}}{2^w_b} \left[ \exp \left( i \sum_{i \in e_X} \theta_i r_i \right) + (-1)^{a_P} \exp \left( -i \sum_{i \in e_X} \theta_i r_i \right) \right] \prod_{j \notin e_X} Q_{a_j} \left(\sum_{i \in e_X} \theta_{ij} r_i \right).
\]

where \(a_P = \sum_{j \notin e_X} a_j \mod 2\). We can now merge the two complex phases to obtain the final expression

\[
\langle Z^a X^b \rangle = \frac{i^{w_a+a_P}}{2^{w_b-1}} \sum_{\{r\}/\mathbb{Z}_2} Q_{a_P} \left(\sum_{i \in e_X} \theta_i r_i \right) \prod_{j \notin e_X} Q_{a_j} \left(\sum_{i \in e_X} \theta_{ij} r_i \right).
\]

This expresses the expectation value as a sum of \(2^{w_b-1}\) terms, and can be computed efficiently when the operators we are interested in have small weight \(w \ll N\). In particular, to perform the optimization of the ansatz as described in the main text, we only make use of this expression with \(w_b\) up to 2. Note that when \(w_b = 0\) we have a vanishing expectation value.

We will now show how Eq. \((A10)\) can be used to efficiently compute the expectation of the Hamiltonian in the SD-IQP
\[ \langle H \rangle_{\theta} = \sum_{i} h_{i} \langle Z_{i} \rangle_{\theta} + \sum_{\langle i,j \rangle} J_{ij} \langle Z_{i} Z_{j} \rangle_{\theta} \]

\[ = \sum_{i} h_{i} (\cos \phi_{i} \langle Z_{i} \rangle - i \sin \phi_{i} \langle Z_{i} X_{i} \rangle) \]

\[ + \sum_{\langle i,j \rangle} J_{ij} (\cos \phi_{i} \cos \phi_{j} \langle Z_{i} Z_{j} \rangle - \cos \phi_{i} \sin \phi_{j} \langle Z_{i} Z_{j} X_{j} \rangle) - \sin \phi_{i} \cos \phi_{j} \langle Z_{i} Z_{j} X_{j} \rangle - \sin \phi_{i} \sin \phi_{j} \langle Z_{i} Z_{j} X_{j} \rangle) \].

(A11)

We may now use Eq. (A10) to expand each term in this expression. First, we note that expectation values with no \(X\) operators simply vanish, so \(\langle Z_{i} \rangle = 0\) and \(\langle Z_{i} Z_{j} \rangle = 0\). Then we can compute the remaining terms individually:

\[ \langle Z_{i} X_{i} \rangle = i \sin \theta_{i} \prod_{l \neq i} \cos \theta_{il}, \]  

(A12)

\[ \langle Z_{i} Z_{j} X_{i} \rangle = i \cos \theta_{i} \sin \theta_{ij} \prod_{l \neq i,j} \cos \theta_{il}, \]  

(A13)

\[ \langle Z_{i} Z_{j} X_{j} \rangle = i \cos \theta_{j} \sin \theta_{ij} \prod_{l \neq i,j} \cos \theta_{lj}, \]  

(A14)

\[ \langle Z_{i} Z_{j} X_{i} X_{j} \rangle = \frac{1}{2} \left[ \cos(\theta_{i} + \theta_{j}) \prod_{l \neq i,j} \cos(\theta_{il} + \theta_{lj}) - \cos(\theta_{i} - \theta_{j}) \prod_{l \neq i,j} \cos(\theta_{il} - \theta_{lj}) \right]. \]  

(A15)

If we plug these expressions into Eq. (A11) we arrive at the final analytic form for our Hamiltonian expectation value:

\[ \langle H \rangle_{\theta} = \sum_{i} h_{i} \sin \phi_{i} \sin \theta_{i} \prod_{l \neq i} \cos \theta_{il} \]

\[ + \sum_{\langle i,j \rangle} J_{ij} \left[ \cos \phi_{i} \sin \phi_{j} \cos \theta_{ij} \prod_{l \neq i,j} \cos \theta_{il} + \sin \phi_{i} \cos \phi_{j} \cos \theta_{ij} \prod_{l \neq i,j} \cos \theta_{il} \right] - \frac{1}{2} \sin \phi_{i} \sin \phi_{j} \left[ \cos(\theta_{i} + \theta_{j}) \prod_{l \neq i,j} \cos(\theta_{il} + \theta_{lj}) - \cos(\theta_{i} - \theta_{j}) \prod_{l \neq i,j} \cos(\theta_{il} - \theta_{lj}) \right] \].

(A16)

Note that the computational time of evaluating this expectation value, as well as the gradient in \(\theta\), is \(O(N^3)\), if the problem Hamiltonian has all to all connectivity, as is the case for the Sherrington-Kirkpatrick model. It can be reduced to \(O(DN^2)\) if our problem can be formulated on a graph whose degree is bounded by \(D\). Analogous efficient expressions may be obtained for problem Hamiltonians that include many-body interactions, as long as the weights scale at most like \(O(\log N)\) with the problem size.

**Appendix B: Derivation of the Gram matrix**

In order to perform VarQITE we must compute the Gram matrix \(A\) corresponding to the tangent vectors of our variational manifold. According to its definition in [21] we have:

\[ A_{\mu \nu} = \text{Re} \left( \frac{\partial \langle \Psi(\theta) \rangle \partial \langle \Psi(\theta) \rangle}{\partial \theta_{\mu} \partial \theta_{\nu}} \right), \]  

(B1)

where we used Greek indices \(\mu, \nu\) that run over all variational parameters in the ansatz. We can now separate this matrix into several blocks based on the type of variational parameter.
A = \begin{bmatrix} A^{\theta\phi} & A^{\phi\theta} \\ A^{\phi\theta} & A^{\theta\theta} \end{bmatrix}. \tag{B2}

From the definition in Eq. (5) we can explicitly compute the tangent vectors as
\[
\frac{\partial \ket{\Psi(\theta)}}{\partial \theta_k} = -\frac{i}{2} \bigotimes_{j \in \mathcal{N}} R_x(\phi_j) X_k \exp(-i \mathcal{H}_{\mathrm{IQP}}) \ket{+}^\otimes N, \tag{B3}
\]
\[
\frac{\partial \ket{\Psi(\theta)}}{\partial \phi_e} = -\frac{i}{2} \bigotimes_{j \in \mathcal{N}} R_x(\phi_j) Z_e \exp(-i \mathcal{H}_{\mathrm{IQP}}) \ket{+}^\otimes N, \tag{B4}
\]
where \( e \) is a subset of \( \mathcal{N} \) present in the IQP ansatz. For the \( \theta\theta \) part of the matrix we get
\[
A^{\theta\theta}_{ee'} = \frac{1}{4} \text{Re}(\langle Z_e Z_{e'} \rangle) = \frac{1}{4} \delta_{ee'}, \tag{B5}
\]
where we again employ the notation \( \langle \cdot \rangle \), which stands for the expectation value in the state \( \exp(-i \mathcal{H}_{\mathrm{IQP}}) \ket{+}^\otimes N \).

This result states that varying the parameters \( \theta_e \) one at a time with the same starting point on the manifold will take us along orthogonal directions. For the \( \theta\phi \) part and \( |e| = 1 \) we have
\[
A^{\theta\phi}_{ik} = \frac{1}{4} \text{Re}(\langle Z_i X_k \rangle) = \begin{cases} 0, & \text{for } k = i \\ -\frac{1}{4} \sin \theta_k \sin \theta_{ik} \prod_{l \neq i,k} \cos \theta_{lk}, & \text{for } k \neq i \end{cases}, \tag{B6}
\]
and for \( |e| = 2 \) we get
\[
A^{\theta\phi}_{(ij)k} = \frac{1}{4} \text{Re}(\langle Z_i Z_j X_k \rangle) = \begin{cases} 0, & \text{for } k = i \text{ or } k = j \\ -\frac{1}{4} \cos \theta_k \sin \theta_{ik} \sin \theta_{jk} \prod_{l \neq i,j,k} \cos \theta_{lk}, & \text{for } k \neq i,j \end{cases}. \tag{B7}
\]

Since \( A \) must be hermitian, we can get the other off-diagonal block matrix as \( A^{\phi\theta} = (A^{\theta\phi})^T \). Finally in the \( \phi\phi \) sector we have
\[
A^{\phi\phi}_{kq} = \frac{1}{4} \text{Re}(\langle X_k X_q \rangle) = \begin{cases} 1/4, & \sum_{s \in \{+1,-1\}} \frac{1}{8} \cos(\theta_i + s \theta_j) \prod_{l \neq i,j} \cos(\theta_{li} + s \theta_{lj}) & \text{for } k = q \\ \frac{1}{8} \sum_{s \in \{+1,-1\}} \cos(\theta_i + s \theta_j) \prod_{l \neq i,j} \cos(\theta_{li} + s \theta_{lj}) & \text{for } k \neq q \end{cases}. \tag{B8}
\]

Appendix C: Energy landscape

In the main text, we claim that, for small problem sizes, we sometimes do not find a non-trivial local minima and instead the ansatz loses its overlap with the ground state. In this case, we still hit a plateau during the optimization and we overcome this issue by choosing to sample the IQP ansatz close to the middle of the plateau. This situation is illustrated in Fig. 5(b). In the attached histogram we see that the state obtained at the end of the optimization (orange) has non-zero support only on a small number of states and does not find the ground state, despite having a much lower average energy. Sampling in the middle of the first plateau (blue) results in a wider spread of states, including a high overlap onto the ground state.

In Fig. 6 we show that the cases where the algorithm does not converge to a good local optima become very unlikely as we increase the number of qubits.

Appendix D: Example of non-trivial minima of the optimization landscape

In this appendix we give a minimal example of a problem for which the IQP ansatz leads to non-trivial local minima, where by non-trivial we mean that the state produced is not an eigenstate of the Hamiltonian. Additionally, the state is shown to have an overlap of 0.5 onto the degenerate ground eigenspace, so the problem solution can be recovered by sampling.
Consider the 4-qubit Hamiltonian

\[ H = Z_0 (Z_1 + Z_2 + Z_3). \]  

We explore this Hamiltonian using the IQP ansatz given by all 1-body and 2-body X operators

\[ H_{\text{IQP}} = \sum_{i=0}^{3} \theta_i X_i + \sum_{\langle i,j \rangle} \theta_{ij} X_i X_j \]  

\[ |\Psi_{\text{IQP}}\rangle = \exp \left( -\frac{i}{2} H_{\text{IQP}} \right) |0\rangle, \]

which is equal to the one in Eq. (4) of the main text.

We compute the expectation value \( \langle Z_0 Z_1 \rangle \) in the IQP state. The other 2 terms in H are obtained by cyclic permutations in 1, 2, 3.

\[ \text{FIG. 5. Energy plot during simple gradient descent, starting from the optimal QAOA parameters for randomly generated 25 qubit optimization problems. a) Nearby non-trivial local minimum is found and probability of sampling the ground state is amplified, b) Ansatz becomes degenerate after long plateau. Orange shows samples collected from the final step and blue shows samples collected in the middle of the first plateau. All histograms are obtained from a total of 200 samples.} \]

\[ \text{FIG. 6. Fraction of problems that reach a local minimum near the starting QAOA position. The degenerate cases illustrated in Fig. 5(b) become very rare as we increase the number of qubits.} \]
\[
\langle Z_0 Z_1 \rangle = \langle 0 | \exp \left( \frac{i}{2} H_{IQP} \right) Z_0 Z_1 \exp \left( -\frac{i}{2} H_{IQP} \right) | 0 \rangle \\
= \langle 0 | \exp \left[ -i (\theta_0 X_0 + \theta_1 X_1 + \theta_{02} X_0 X_2 + \theta_{03} X_0 X_3 + \theta_{12} X_1 X_2 + \theta_{13} X_1 X_3) \right] | 0 \rangle.
\]

(D4)

Since all terms in the exponential commute, we can expand each factor individually as

\[
\langle Z_0 Z_1 \rangle = \langle 0 | (\cos \theta_0 - i \sin \theta_0 X_0) \cdots (\cos \theta_{13} - i \sin \theta_{13} X_1 X_3) | 0 \rangle.
\]

(D5)

The only terms that survive are those that multiply to identity. The 4 products with this property are \(I\), \(X_0(X_0 X_3)(X_3 X_1) X_1\), \(X_0(X_0 X_3)(X_3 X_1) X_1\), \((X_0 X_2)(X_2 X_1)(X_1 X_3)(X_3 X_0)\). Then we have

\[
\langle Z_0 Z_1 \rangle = \cos \theta_0 \cos \theta_1 \cos \theta_{02} \cos \theta_{03} \cos \theta_{12} \cos \theta_{13} + \\
+ \sin \theta_0 \sin \theta_1 \cos \theta_{02} \sin \theta_{03} \cos \theta_{12} \sin \theta_{13} + \\
+ \sin \theta_0 \sin \theta_1 \sin \theta_{02} \cos \theta_{03} \sin \theta_{12} \cos \theta_{13} + \\
+ \cos \theta_0 \cos \theta_1 \sin \theta_{02} \sin \theta_{03} \sin \theta_{12} \sin \theta_{13}.
\]

(D6)

We provide a symbolic implementation of this expression in Python [32]. Using symbolic differentiation, we show that the line given by equations \(\theta_0 = \pi/2, \theta_1 = \pi/2, \theta_3 = \pi/2, \theta_{01} = \pi/2, \theta_{02} = \pi, \theta_{12} = 0, \theta_{03} = \pi/2, \theta_{13} = \pi/2, \theta_{23} = 0\) (note that \(\theta_2\) is free and parameterizes the line) is a critical line of local minima. This is done by verifying that the gradient is 0 for all \(\theta_2\) and the Hessian is positive semi-definite, with a single null eigenvalue corresponding to the direction going along the curve (except at the isolated point \(\theta_2 = \pi/2\) which we exclude from our analysis). In addition, the expected value of the Hamiltonian on this line is \(\langle H \rangle = -2\), while it is easy to check that all eigenvalues of the Hamiltonian must be odd integers. Therefore, the states created by the ansatz with the specified parameters must be superposition of eigenstates with different eigenvalues. We claim that this is sufficient to show that all points on the line are non-trivial local minima and give the following proof:

**Proof.** Consider an optimization space parameterized by \((\phi, \tilde{\theta})\) variables, with the usual parameter range of 0 to 2\(\pi\). Let us call the cost function defined on this space by \(J(\phi, \tilde{\theta})\). Assume \(J\) is infinitely smooth, so we can freely Taylor expand around all points (this can be verified from the analytic form of \(J\) in terms of sums of products of smooth functions). Assume the line of critical points found in the counterexample is defined by the condition \(\tilde{\theta} = \tilde{\theta}_0\) for some constant \(\tilde{\theta}_0\). \(\phi\) can then be considered a parameterization of the critical line (changing its value moves us along the line). On this line we showed that the cost function is constant

\[
J(\phi, \tilde{\theta}_0) = -2,
\]

and the gradient is 0

\[
\nabla J(\phi, \tilde{\theta}_0) = 0.
\]

(D8)

At Hessian level we find that all second order derivatives that contain \(\phi\) are zero

\[
\partial_{\theta_i} \partial_{\theta_j} J(\phi, \tilde{\theta}_0) = 0,
\]

\[
\partial_{\phi}^2 J(\phi, \tilde{\theta}_0) = 0,
\]

(D9) (D10)

and the restriction of the Hessian to the \(\tilde{\theta}\) subspace is positive definite on some interval \([\phi_\prec, \phi_\succ]\) with \(0 < \phi_\prec < \phi_\succ < \pi/2\):

\[
v_i \partial_{\theta_i} \partial_{\theta_j} J(\phi, \tilde{\theta}_0) v_j > 0
\]

(D11)

for all nonzero vectors \(v\) and \(\phi \in [\phi_\prec, \phi_\succ]\). Einstein summation convention is employed. In particular, for all unit vectors \(\hat{n}\) we have that
\begin{align}\label{eq:12}
d_i \partial \theta_i \partial \theta_j J(\phi, \tilde{\theta}_0) n_j \geq \lambda_{\text{min}}(\phi) > 0,
\end{align}

with \(\lambda_{\text{min}}(\phi)\) the smallest eigenvalue of the Hessian at \((\phi, \tilde{\theta}_0)\) when restricted to the \(\theta_i\) variables.

Note that the role of \(\phi\) is played by \(\theta_2\) in our example, but we changed the name for brevity. Suppose we want to focus our attention on the point \((\phi_0, \tilde{\theta}_0)\) with \(\phi_0 \in [\phi_-, \phi_+]\) and show that this is indeed a local minimum. The coordinates of every point in the vicinity of this critical point that do not lie on the critical line can be written as \((\phi_0 + \epsilon \Delta \phi, \tilde{\theta}_0 + \epsilon \Delta \tilde{\theta})\), where \(\Delta \tilde{\theta}\) is a unit vector and \(\epsilon\) is some small quantity. We can write the value of the cost function at this point as

\begin{align}\label{eq:13}
J(\phi_0 + \epsilon \Delta \phi, \tilde{\theta}_0 + \epsilon \Delta \tilde{\theta}) = J(\phi_0 + \epsilon \Delta \phi, \tilde{\theta}_0) +
\frac{\epsilon^2}{2} \Delta \theta_i \Delta \theta_j \partial \theta_i \partial \theta_j J(\phi_0 + \epsilon \Delta \phi, \tilde{\theta}_0) + R(\epsilon),
\end{align}

where from the theory of Taylor series we know that \(R(\epsilon)\) is continuous and

\begin{align}\label{eq:14}
\lim_{\epsilon \to 0} \frac{R(\epsilon)}{\epsilon^2} = 0.
\end{align}

The linear term in the equation above has been dropped due to Eq. \[\text{[D8]}\] stating that all points of \(\tilde{\theta} = \tilde{\theta}_0\) have vanishing gradients. Since the cost function is constant under shifts in \(\phi\) this is equivalent to

\begin{align}\label{eq:15}
J(\phi_0 + \epsilon \Delta \phi, \tilde{\theta}_0 + \epsilon \Delta \tilde{\theta}) - J(\phi_0, \tilde{\theta}_0) =
\frac{\epsilon^2}{2} \Delta \theta_i \Delta \theta_j \partial \theta_i \partial \theta_j J(\phi_0 + \epsilon \Delta \phi, \tilde{\theta}_0) + \frac{R(\epsilon)}{\epsilon^2} \geq \frac{1}{2} \lambda_{\text{min}}(\phi_0 + \epsilon \Delta \phi) + \frac{R(\epsilon)}{\epsilon^2}.
\end{align}

Since the minimum eigenvalue is strictly positive in the \(\tilde{\theta}\) subspace and \(R(\epsilon)/\epsilon^2\) is a continuous function that decays to 0 for \(\epsilon \to 0\) we conclude that there must exist some \(\epsilon_0 > 0\) such that that RHS of the above inequality is strictly positive for all \(|\epsilon| < \epsilon_0\). Since this implies that the LHS must also be positive for all values of \(\epsilon\) in this ball around 0, then this proves that the value of the cost function in the neighborhood must be strictly larger than its value on the critical line. The above prescription can be applied to all perturbations around the critical point except those with \(\Delta \tilde{\theta} = 0\), for which we know that the cost function must be constant. This proves that all points on the critical line represent local minima (similar to the minima of the Mexican hat potential).