Space-efficient binary optimization for variational computing

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Abstract

In the era of Noisy Intermediate-Scale Quantum (NISQ) computers it is crucial to design quantum algorithms which do not require many qubits or deep circuits. Unfortunately, the most well-known quantum algorithms are too demanding to be run on currently available quantum devices. Moreover, even the state-of-the-art algorithms developed for the NISQ era often suffer from high space complexity requirements for particular problem classes.

In this paper, we show that it is possible to greatly reduce the number of qubits needed for the Travelling Salesman Problem (TSP), a paradigmatic optimization task, at the cost of having deeper variational circuits. While the focus is on this particular problem, we claim that the approach can be generalized for other problems where the standard bit-encoding is highly inefficient. Finally, we also propose encoding schemes which smoothly interpolate between the qubit-efficient and the circuit depth-efficient models. All the proposed encodings remain efficient to implement within the Quantum Approximate Optimization Algorithm framework.

1 Introduction

During the past few decades, a wealth of quantum algorithms have been designed for various problems, many of which offered a speedup over their classical equivalents [1, 2, 3, 4]. The theoretical developments have also been complemented by progress on the experimental side. Indeed, the demonstration of quantum supremacy by Google [5] indicates that in the near future useful quantum technology may be available. However, current Noisy Intermediate-Scale Quantum (NISQ) devices are too small and too noisy to implement complicated algorithms like Shor’s factorization algorithm [2] or Grover-search based optimizers [6, 7]. This resulted in a new field of quantum computation which focuses on designing new algorithms requiring significantly less noisy qubits.

Optimization is a problem which seems to be particularly suitable for current NISQ devices. In particular, the Variational Quantum Eigensolver (VQE) [8, 9, 10] seems to be the state-of-the-art algorithm for solving molecule Hamiltonians. Although it can solve optimization problems defined over discrete spaces, so-called combinatorial optimization problems, quantum annealing and Quantum Approximate Optimization Algorithm (QAOA) [11] are considered to be more suitable.

For all of these algorithms, the original combinatorial optimization problem has to be transformed into the Ising model. Typically, one starts with a high-level description, like the Max-Cut problem, where nodes in the graph $G = (V,E)$ have to be colored either red or black, so that certain function is minimized. Then, one has to transform it to a pseudo-Boolean polynomial $\sum_{\{u,v\} \in E} (b_u - b_v)^2$. Each binary variable (bit) $b_v$ denotes the color of the node $v$ in the graph. For example we can choose $b_v = 1$ for red color, and $b_v = 0$ for black color. For quantum algorithms it is convenient to change the representation into Ising model via transformation $b_v \leftarrow (1 - Z_v)/2$. Here $Z_v$ is a Pauli operator acting on a qubit corresponding to the node $v$. By transforming the original objective function into Hamiltonian, we also change the domain of the problem into the space of quantum states.

Quantum optimization algorithms differ in the way how they solve the problem. Variational Quantum Eigensolver (VQE) is a heuristic algorithm in which the quantum cir-
cuit is optimized using classical procedure. More precisely, we are given an *ansatz* \( U(\theta) \) which, after fixing the parameter \( \theta \), produces a state \( |\theta\rangle = \prod_{i=1}^{k} U_i(\theta_i) |0\rangle \). The vector \( \theta \) is optimized using classical optimization procedure like gradient descent or simultaneous perturbation stochastic approximation (SPSA), so that \( |\theta\rangle \) will be localized at high quality answer. Due to its generality, VQE is commonly used for molecule Hamiltonians, however its usability to the classical optimization problems may be limited.

Quantum annealing theoretically can also be applied for chemistry Hamiltonians, however current machines restrict their usability to combinatorial optimization problems. The algorithm turns the ground state of initial Hamiltonian \( H_{\text{mix}} = \sum_i X_i \) into a ground state of objective Hamiltonian \( H \) through adiabatic evolution \( g(t)H_{\text{mix}}+(1-g(t))H \). Adiabatic theorem provides a good premise for high-quality solutions of the problem. Furthermore, while available D-Wave’s annealers have thousands of qubits, the topology restrictions may limit the size of tractable problems to cases solvable by classical procedures \cite{D-Wave1, D-Wave2}.

Quantum Approximate Optimization Algorithm (QAOA) is a mixture of the methods described above \cite{QAOA}. While quantum annealing is a continuous process, QAOA interchangeably applies both \( H_{\text{mix}} \) and \( H \) for some time. The evolution time is a parameter of the evolution, and as it was in the case of VQE, they are adjusted by external classical procedure. Here the resulting state takes the form

\[
|\theta\rangle = \prod_{i=1}^{r} \exp(-i\theta_{\text{mix},i}H_{\text{mix}}) \exp(-i\theta_{\text{obj},i}H) |+\rangle,
\]

where \( r \) is the number of levels. The algorithm can be implemented as long as both mixing and objective Hamiltonians can be implemented, which in particular allows for applying it to combinatorial problems. Many studies have been performed to characterize properties of QAOA algorithms, including, both rigorous proofs of computational power and reachability properties \cite{QAOA1, QAOA2, QAOA3, QAOA4} as well as characterization through heuristics and numerical experiments and extensions of the algorithm \cite{QAOA5, QAOA6, QAOA7, QAOA8}.

While the proposed quantum algorithms can theoretically solve arbitrary combinatorial optimization problems, not all pseudo-Boolean polynomials can be natively considered for current quantum devices. A general pseudo-Boolean polynomial takes the form

\[
H(b) = \sum_{I \subseteq \{1, \ldots, n\}} \alpha_I \prod_{i \in I} b_i,
\]

where \( \alpha_I \in \mathbb{R} \) defines the optimization problem. An order of such Hamiltonian is a maximum size of \( S \) for which \( \alpha_S \) is nonzero. Current D-Wave machines are restricted to polynomials of order 2, hence if one would like to solve Hamiltonians of higher order, first a quadratization procedure has to be applied, in general at cost of extra qubits \cite{Quadratization}. Note that optimization of quadratic polynomials, Quadratic Unconstrained Binary Optimization (QUBO) is NP-complete, hence it encapsulates most of the relevant problems.

The objective Hamiltonian for Max-Cut requires \( n \) qubits for graph of order \( n \). Hence it can encode \( 2^n \) solutions, which is equal to the number of all possible colorings. However, this is not the case in general. For example for Traveling Salesman Problem (TSP) over \( N \) cities, the QUBO requires \( N^2 \) bits \cite{TSP}. However, \( N! \) permutations requires only \( \left\lfloor \log_2(N!) \right\rfloor \approx N \log N \) bits. We consider this as a waste of computational resources. Unfortunately, in general polynomials with optimal number of qubits have order larger than two, thus we are actually dealing with higher-order binary optimization, which is currently not possible using D-Wave machines.

The idea of using higher-order terms is not new. In fact, in the original work of Farhi et al. \cite{QAOA}, the authors have not restricted the model to two-local model. Furthermore, Hamiltonian of order 4 was used for variational quantum factoring \cite{QAOA1}, while Hamiltonian of order \( l \) was constructed for Max-\( l \)-SAT problem \cite{QAOA5}. Since the terms of arbitrary order can be implemented efficiently, QAOA for the problem can reduce the number of required logical qubits. In general, if objective polynomial is of constant order \( \alpha \), then the circuit of order \( \mathcal{O}(\binom{n}{\alpha} \log \alpha) \) implements the objective Hamiltonian exactly. While the number may be large, it is still polynomial, which makes the implementation tractable. However, even for slowly growing \( \alpha \) (say \( \mathcal{O}(\log n) \)), in general the number of terms grows exponentially, which could be the case for \( l \to \infty \) in Max-\( l \)-SAT. Note that even an encoding that requires only logarithmic number of qubits has been introduced \cite{QAOA2}, however, the minimizer of this encoding does not necessarily map to the minimizer of the original problem.

Furthermore, when dealing with unbounded order, one has to be careful when transforming QUBO into the Ising model. Let us consider a polynomial \( 2^n \prod_{i=1}^{n} b_i \). Using default transformation \( b_i \leftarrow (1 - Z_i)/2 \) will produce Hamiltonian \( \sum_{I \subseteq \{1, \ldots, n\}} (-1)^{|I|} \prod_{i \in I} Z_i \), which consists of \( 2^n \) terms \cite{QAOA2}. For this example, one can easily find a better Hamiltonian \(- \sum_{i=1}^{n} Z_i\), that shares the same global minimizer, however, in general finding such a transforma-
tion requires a higher-level understanding of the problem. Note that this is not an issue for constant-order polynomials, as the number of terms is guaranteed to be polynomial even in the worst case scenario.

Despite the potential issues coming from utilizing unbounded-order polynomials, we present a polynomial (encoding) for TSP problem with unbounded order, which can be efficiently implemented using approximately optimal number of qubits. Furthermore, our model requires fewer measurements for estimating energy. We also developed a transition encoding, where one can adjust the improvement in the required number of qubits and circuit’s depth. Finally, QAOA optimizes our encoding with similar or better efficiency compared to the state-of-the-art QUBO encoding of TSP.

State-of-the-art TSP encoding Current state-of-the-art encoding of TSP problem can be found in the paper by Lucas [23]. Let us consider the Traveling Salesman Problem (TSP) over \( N \) cities. Let \( W \) be a cost matrix, and \( b_t \) be a binary variable such that \( b_{ti} = 1 \) iff the \( i \)-th city is visited at time \( t \). The QUBO encoding takes the form

\[
H^{\text{QUBO}}(b) = A_1 \sum_{t=1}^{N} \left( 1 - \sum_{i=1}^{N} b_{ti} \right)^2 + A_2 \sum_{i=1}^{N} \left( 1 - \sum_{t=1}^{N} b_{ti} \right)^2 + B \sum_{i,j=1 \atop i \neq j}^{N} W_{ij} \sum_{t=1}^{N} b_{ti} b_{t+1,j}.
\]

Here \( A_1, A_2 > B \max_{i \neq j} W_{ij} \) are parameters that have to be adjusted during the optimization. We also assume \( N + 1 \rightarrow 1 \) simplification for the indices. Note that any route can be represented in \( N \) different ways, depending on which city is visited at time \( t = 1 \). Such redundancy can be solved by fixing that the first city should be visited at time \( t = 1 \). Thanks to that, \( n = (N - 1)^2 \) (qu)bits in total are required.

In the scope of this paper we will take advantage of various quality measures of encodings. First, since the Hamiltonian has to be implemented directly, we prefer encodings with possibly small depth. In this manner, QUBO can be efficiently implemented using approximately optimal number of qubits. Furthermore, our model requires significantly smaller than \( N^2 \). Note that the number of qubits also has an impact on the volume of the circuit, traditionally defined as a product of the number of qubits and the circuit’s depth. In case of this encoding the volume is of order \( O(N^3) \).

Finally, in the paper we also consider the required number of measurements to estimate the energy within constant additive error. Instead of estimating each term of the Hamiltonian independently, which has to be done for VQE, we consider the measurement’s output as a single sample. This way, using Hoeffding’s theorem, QUBO encoding requires \( O(N^3) \) measurements.

Results

Preliminaries Traveling Salesman Problem is natively defined over the permutations of \( \{1, \ldots, N\} \). A simple encoding can be defined as follows. We make a partition of all bits into \( N \) collections \( b_t \), where each collection encodes a city visited in a particular time. Then, for each collection we choose a number encoding which represents the city.

QUBO is an example of such an encoding, where each city is represented by an one-hot vector, see Fig. 1. Instead, each city can be encoded as a number using binary numbering system. Using numbering system is a state-of-the-art way to encode inequalities [23], however it is new in the context of encoding elements of a feasible space.

The Hamiltonian takes the form

\[
H(b) = A_1 \sum_{t=1}^{N} H^{\text{valid}}(b_t) + A_2 \sum_{t=1}^{N} \sum_{t'=t+1}^{N} H_{\#}(b_t, b_{t'}) + B \sum_{i,j=1 \atop i \neq j}^{N} W_{ij} \sum_{t=1}^{N} H_{\delta}(b_t, i) H_{\delta}(b_{t+1}, j).
\]

Hamiltonian \( H^{\text{valid}} \) checks whether a vector of bits \( b_t \) encodes a valid city. For example for QUBO it checks whether at most one bit is equal to 1. Hamiltonian \( H_{\#} \) verifies whether two collections encode the same city. Note that QUBO encoding falls into this representation by choosing

\[
H_{\#}^{\text{QUBO}}(b_t, b_{t'}) = \sum_{i,j} \left( 2b_{ti}b_{t'j} + \frac{1}{(2)}(1 - b_{ti} - b_{t'j}) \right).
\]

Hamiltonian \( H_{\delta} \) plays a similar role as \( H_{\#} \). If the inputs are different, then both \( H_{\delta} \) and \( H_{\#} \) give zeros. If the inputs are the same, then the outputs are nonzero and moreover we expect that the Hamiltonian \( H_{\#} \) outputs 1.
Figure 1: Visualization of QUBO encoding and encodings introduced in the paper for TSP problem. a) exemplary solution for TSP problem. On the right there are assignments of the exemplary solution using respectively b) QUBO, c) HOBO d), naive mixed, and e) mixed encodings.

Figure 2: Round-robin schedule [27] for binary vectors $b_1, \ldots, b_5$. We assumed that each $b_i$ is defined over 3 qubits. Each gate defined over a pair $b_i, b_j$ is an implementation of the Hamiltonian defined over these variables. Such Hamiltonian can be implemented using the technique visualized in Fig. [3]
This is in order to preserve the costs of routes. In case of QUBO we took $H_3(b_i, i) = b_{i4}$. Note that in particular $H_3 = H_{\phi}$ may be a good choice, however later we will show that choosing different $H_{\phi}$ may be beneficial.

Simple HOBO encoding  The simplest encoding is the one in which each collection $b_t$ encodes a city in a binary system, see Fig. 1. In this case, for each time we need $K := \lceil \log N \rceil$ qubits. In total we need $\sim N \log(N)$ qubits, which match the lower bound. Moreover, we have to design $H_{\text{valid}}$ in such a way that $b_t$ represents the number at most $N - 1$.

Following Eq. 2, it is easy to note that HOBO defined in a way described above, is of polynomial size. Note that the sum of Hamiltonians $H_t$ produces at most $(N)^2K$ elements. Furthermore, the terms introduced by $H_{\text{valid}}$ and $H_{\phi}^{\text{HOBO}}$ are already present in $H_{\phi}^{\text{HOBO}}$. Hence in total we have $\mathcal{O}(N^4)$ terms, which implies the polynomial size and depth, and thus volume.

Let us now present an exemplary encoding. Suppose $\tilde{b}_{K-1} \ldots \tilde{b}_0$ is a binary representation of $N - 1$. Suppose $k^0 \in K_0$ are such indices that $\tilde{b}_{k^0} = 0$. Then one can show that

$$H_{\text{valid}}^{\text{HOBO}}(b_t) := \sum_{k^0 \in K_0} \left( b_{k^0} \prod_{k=k^0+1}^{K-1} (1 - (b_{t,k} - \tilde{b}_k)^2) \right)$$

validates whether the encoding number is at most $N - 1$. A detailed proof can be found in Supplementary materials, here let us consider an example. Suppose $N - 1 = 100101_2$. All the numbers larger than $N - 1$ are of the form 11?????2 or 101????2, where '?' denotes at arbitrary bit value.

The polynomial

$$b_{t5}b_{t4} + b_{t5}(1 - b_{t4})b_{t3} + b_{t5}(1 - b_{t4})(1 - b_{t3})b_{t2}b_{t1}, \quad (3)$$

punishes all these forms. At the same time, one can verify that numbers smaller than $N - 1$ are not punished by the Hamiltonian.

Here, we will consider $H_{\phi}^{\text{HOBO}} \equiv H_{\phi}^{\text{HOB}}$, hence it is enough to define the latter only. Hamiltonian $H_{\phi}^{\text{HOB}}$ can be defined as

$$H_{\phi}^{\text{HOB}}(b_t, b'_t) := \sum_{k=1}^{K} (1 - (b_k - b'_k)^2).$$

Note that if $b'$ is a fixed number like it is in the case of objective function implementation in Eq. 2, then we simply take consecutive bits from binary representation.

Let us estimate the cost of this encoding. As it was previously stated, the number of factors is of order $\mathcal{O}(N^4)$. Using round-robin techniques and Gray code, see Fig. 2 and 3 one can show that the depth of the circuit is $\mathcal{O}(N^3)$, which gives us the volume $\mathcal{O}(N^4 \log(N))$. Note that the Gray code requires additional $\lceil NK/2 \rceil$ qubits, which does not change the final result. Finally, in order to achieve a similar quality of energy measurements, we need $\mathcal{O}(N^2)$ measurements.

One can expect that higher-order binary optimization may lead to difficult landscapes, harder to investigate for optimization algorithm. We have investigated TSP encodings with $W \equiv 0$ and random $W$ matrices. The results are presented in Fig. 4. One can see that with the same number of Hamiltonians applied, the results are either similar or in favor for higher-order encodings.

Mixed QUBO-HOBO approach  While QUBO encoding requires significantly more qubits compared to HOBO, the latter produces much deeper circuits. It is not clear whether the number of qubits or the depth of the circuit will be more challenging, and in fact we claim that both may produce significant difficulties when designing quantum computers.

One can consider a simple mixing of the proposed QUBO and HOBO encodings in the following way: let $R \in \{1, \ldots, N\}$ be a free parameter of our model. Exactly $R$ of collections $b_t$ will be encoded as one-hot vectors (in QUBO’s fashion), while the remaining $N - R$ collections will be encoded using the binary representation, see Fig. 1d.

Unfortunately, this approach combines flaws of both models introduced before. For $R = \Omega(N)$, the mixed approach requires $\Theta(N^2)$ qubits. On the other hand, for $R = \mathcal{O}(N)$ the depth of the circuit is the same as in the HOBO approach due to numerous HOBO-encoded $b_t$.

Instead, we propose another encoding. Suppose $N = (2^K - 1)L$ for suitable integers $K$ and $L$. Each $b_t$ consists of $KL$ qubits of the form $b_{t,k}$. The cities are encoded as follows. First $K$ qubits (first bunch) decodes numbers $1, \ldots, 2^K - 1$. The second bunch decodes $2^K, \ldots, 2^{K} - 2$, and so on. Note that QUBO and HOBO encodings introduced before are special instances with $L = N$ and $L = 1$ respectively.

We add the following assumptions, which also define $H_{\text{valid}}$. All bits being zero is an invalid assignment, which is equivalent to $\sum_{k,t} b_{tk} \geq 1$. This can be forced by using standard techniques for transforming inequalities to QUBO [23]. Secondly, if in some bunch there are nonzero
Figure 3: On the left, two decompositions of $\exp(itZ_1Z_2Z_3)$, a) without auxiliary qubit [28] (p.30), and b) with auxiliary qubit [29] (p.210). On the right, an example of simplifying circuit for $\sum_{I \subseteq \{1,2,3\}} \alpha_I \prod_{i \in I} b_i$ using Gray codes, c) using $Z$ operations only, and d) with CNOTs and single-qubit gates only. In all the figures blue gates are $k$-local $Z$ operations.

Figure 4: The dependence between the probability of measuring the state in feasible space for a) 3 cities, b) 4 cities, c) 5 cities for $W \equiv 0$, and d) 3 cities, e) 4 cities, f) 5 cities for randomly chosen $W$. For most cases HOBO and QUBO present similar quality, while for e) HOBO clearly outperforms QUBO approach. Vertical line denotes the change of optimization method. For f) we were only capable of estimating up to 10 oracles applied due to convergence issues.
bits, then in all other bunches bits have to be zeros. Note that this assumption is equivalent to the fact that for all \( l_0 = 1, \ldots, L \) we have that either \( \sum_k b_{t_0,k} \) is zero or \( \sum_{l_0 \neq l} \sum_k b_{l,k} \) is zero. The Hamiltonian \( H_{\text{valid}}^{\text{MIX}} \) takes the form

\[
H_{\text{valid}}^{\text{MIX}}(b_t) := \left( - \sum_{l=1}^L \sum_{k=0}^{K-1} b_{l,k} + 1 + \sum_{i=0}^{\lceil \log(KL) \rceil} 2^i \xi_{t,i} \right)^2 + \sum_{l=1}^L \left( \sum_{k=0}^{K-1} b_{l,k} \right) \left( \sum_{l' \neq l} \sum_{k=0}^{K-1} b_{l',k} \right).
\]

Here \( \xi_i \) are additional bits for encoding the first assumption. In total, there will be additional \( N \log(KL) \leq N \log(N) \) qubits.

Now let us define \( H_{\phi}^{\text{MIX}} \) Hamiltonian. Since due to \( H_{\text{valid}}^{\text{MIX}} \) there exist two indices \( l_0, l_0' \) such that \( b_{t_0,k} \) and \( b_{t_0',k} \) are nonzero, we only have to check for consecutive bunches \( l = 1, \ldots, L \) if there exists \( l \) such that \( b_{t,l} \) are nonzero and identical. The Hamiltonian \( H_{\phi}^{\text{MIX}} \) takes the form

\[
H_{\phi}^{\text{MIX}}(b_t, b_{t'}) := \sum_{l=1}^L \left( \sum_{k=0}^{K-1} (b_{l,k} + b_{l',k}) \right) \times \prod_{k=1}^K (1 - (b_{l',l,k} - b_{t,l,k})^2).
\]

Note that the first factor checks whether the bunches are nonzero, while the latter is the Kronecker delta implementation as before.

Finally, let us define \( H_b^{\text{MIX}} \). Let \( \bar{l} : \{1, \ldots, N\} \mapsto \{1, \ldots, L\} \) be a function which outputs a bunch index denoting the \( i \)-th city. Then it is enough to apply the Kronecker delta on \( \bar{l}(i) \)-th bunch. Hence \( H_b^{\text{MIX}} \) will take the form

\[
H_b^{\text{MIX}}(b_t, i) := \prod_{k=1}^K (1 - (b_{t,l(i),k} - b_{k}^b))^2,
\]

where \( b_k^b \) is \( k \)-th bit of binary representation of \( i \).

Let us now calculate the efficiency of the encoding. We will consider only the scenario \( k = \alpha \log(N) \) for \( \alpha \in (0, 1) \). First we note that \( L = \frac{N}{\alpha} = \Theta(N^{1-\alpha}) \). For the proposed mixed encoding, we need \( NK + \log(N) \) qubits. Hamiltonian can be encoded in a circuits of depth \( \mathcal{O}(N^{1+2\alpha}) \). This finally gives us the volume \( \mathcal{O}(N^{3-\alpha} \log(N)) \). All this parameters show a perfect, up to poly-log factors, transition between HOBO and QUBO approaches. Finally, to achieve constant error of energy estimation, we require \( \mathcal{O}(N^{3-\alpha} \log(N)) \max_{i \neq j} W_{ij} \) runs of the circuit.

**Optimal encoding** So far we assumed that all binary variables are split into collections of binary variables, such that each collection defines a particular time point. We heavily used this assumption, so that the encoding was particularly simple. Theretofore it was implementable on a quantum computer, which is necessary for QAOA. Nevertheless, dropping this assumption can save us from even more qubits.

Let \( H \) be a diagonal Hamiltonian. Then \( \langle \psi | H | \psi \rangle = \sum_{\alpha \in \{0, 1\}^n} E_\alpha \langle \beta(\psi) | 2^\alpha \rangle \), where \( E_\alpha \) is the energy value corresponding to the bit string \( \alpha \). Hence, the statistics from the measurements are sufficient to estimate the energy.

Suppose we are given a general combinatorial optimization problem of function \( f : A \to \mathbb{R} \), where \( A \) is a natural feasible space for the problem. In the case of TSP, \( A \) would be a collection of all permutations of some fixed order. Let \( g : A \to B = \{0, 1\}^n \) be a bijection function where \( n = \lceil \log(|A|) \rceil \). Let \( g_{\text{inv}}(b) \) be an extension of \( g^{-1} \) such that it maps some penalty energy \( E_{\text{pen}} > \min_{a \in A} f(a) \), i.e. \( g_{\text{inv}}(b) = g^{-1}(b) b \in B + E_{\text{pen}} \delta_{b \in B} \). Then provided that \( g_{\text{inv}} \) can be efficiently computed, we can use it to estimate the expected energy directly from the measurement’s statistics. Since converting binary representation into numbers takes negligible time, it is enough to provide a procedure for numbering elements of \( A \).

We can incorporate this technique to TSP problem as well. In this case the simplest way is to use a factorial numbering system in which \( i \)-th digit starting from least significant can be any number between 0 and \( i - 1 \). In general \( (d_0, \ldots, d_0) \equiv \sum_{i=0}^k d_i \cdot i! \). The opposite transformation can be done by computing the modulo by consecutive natural numbers. Then such representation can be transferred to permutation via Lehmer codes, which starting with the most significant factoradic digit, take \((k + 1)\)-th digit of the sequence \( (0, 1, \ldots, k) \). The used digit is removed and the procedure repeats for next digits. The taken digits in given order directly encodes a permutation.

Since the procedure described above maps consecutive natural numbers to routes, we require only \( \lceil \log(N!) \rceil \) qubits, which is optimal for each \( N \). Since arbitrary pseudo-Boolean function can be transformed to pseudo-Boolean polynomial, it is as well the case for \( f \circ g_{\text{inv}} \). Hence there exists a diagonal Hamiltonian representing the same optimization problem. However, in general such encoding may require exponential number of terms, which makes it
Note that the approach cannot be applied for general \( H \)-OBO and mixed approaches. According to Eq. (2) we can split all the terms into those defined over pairs \((b_t, b_{t'})\) for \( t \neq t' \). For pairwise different \( t_0, t_1, t_2, t_3 \), if we have polynomials defined over \( b_{t_0}, b_{t_1}, \) and \( b_{t_2}, b_{t_3} \), then we can implement them independently. Using round-robin schedule, we can implement those \( \binom{N}{2} \) polynomials in \( N - 1 \) \((N)\) steps for even (odd) \( N \), as it is described in Fig. 2.

Let \( H \) be a general Hamiltonian defined over \( K \) bits. If we implemented each term independently, then it would require \( \sum_{k=1}^{K} 2^{\binom{k}{2}} \Theta(2^K K) = 2^K K - 1 \) controlled NOTs according to the decomposition presented in Fig. 3b). Adding single auxiliary qubit and using the decomposition from Fig. 3b), and ordering terms according to Gray code, we can do it using \( 2^K \) qubits. Following the reasoning from previous paragraph we can apply only \( \lceil \frac{N}{2} \rceil \) Hamiltonians at once. We have an additional cost of \( \lceil \frac{N}{2} \rceil \) qubits, however reducing the depth cost by \( K = \Theta(\log n) \) for both mixed and simple HOBO approaches.

As far as QUBO is concerned, we have to make separate analysis, since only 2-local terms are present. Note that 1-local terms \( Z_{i;i} \) can be implemented with circuit of depth 1. Moreover, for each \( 1 \leq t \leq N \), terms \( \{ Z_{i;i} Z_{t;i} : 1 \leq i < j \leq N \} \) can be implemented with a circuit of depth \( N \) using round-robin schedule. We can similarly implement \( \{ Z_{i;i} Z_{t;i} : 1 \leq t < t' \leq N \} \), which implement first two addends of \( H^{QUBO} \). For the last addend we have to implement for each \( 1 \leq t \leq N \) terms \( Z = \{ Z_{i;i} Z_{t;i} : i < j \} \). First note that we can first implement them for even \( t \), then for odd \( t \), which doubles the depth of the circuit for single \( t \). Finally, note that \( Z = \bigcup_{k=1}^{N-1} Z_k \), where each \( Z_k = \{ Z_{i;i} Z_{t+i;i+k} : 1 \leq i < N \} \) can be implemented with circuit of depth 1. Eventually, the depth of Hamiltonian \( H^{QUBO} \) is of order \( \Theta(N) \).

The detailed analysis for each encoding can be found in Supplementary materials.

### Methods

#### The analysis of circuits’ depths

Let us begin with HOBO and mixed approaches. According to Eq. (2) we can split all the terms into those defined over pairs \((b_t, b_{t'})\) for \( t \neq t' \). For pairwise different \( t_0, t_1, t_2, t_3 \), if we have polynomials defined over \( b_{t_0}, b_{t_1}, \) and \( b_{t_2}, b_{t_3} \), then we can implement them independently. Using round-robin schedule, we can implement those \( \binom{N}{2} \) polynomials in \( N - 1 \) \((N)\) steps for even (odd) \( N \), as it is described in Fig. 2.

Let \( H \) be a general Hamiltonian defined over \( K \) bits. If we implemented each term independently, then it would require \( \sum_{k=1}^{K} 2^{\binom{k}{2}} \Theta(2^K K) = 2^K K - 1 \) controlled NOTs according to the decomposition presented in Fig. 3b). Adding single auxiliary qubit and using the decomposition from Fig. 3b), and ordering terms according to Gray code, we can do it using \( 2^K \) qubits. Following the reasoning from previous paragraph we can apply only \( \lceil \frac{N}{2} \rceil \) Hamiltonians at once. We have an additional cost of \( \lceil \frac{N}{2} \rceil \) qubits, however reducing the depth cost by \( K = \Theta(\log n) \) for both mixed and simple HOBO approaches.

As far as QUBO is concerned, we have to make separate analysis, since only 2-local terms are present. Note that 1-local terms \( Z_{i;i} \) can be implemented with circuit of depth 1. Moreover, for each \( 1 \leq t \leq N \), terms \( \{ Z_{i;i} Z_{t;i} : 1 \leq i < j \leq N \} \) can be implemented with a circuit of depth \( N \) using round-robin schedule. We can similarly implement \( \{ Z_{i;i} Z_{t;i} : 1 \leq t < t' \leq N \} \), which implement first two addends of \( H^{QUBO} \). For the last addend we have to implement for each \( 1 \leq t \leq N \) terms \( Z = \{ Z_{i;i} Z_{t;i} : i < j \} \). First note that we can first implement them for even \( t \), then for odd \( t \), which doubles the depth of the circuit for single \( t \). Finally, note that \( Z = \bigcup_{k=1}^{N-1} Z_k \), where each \( Z_k = \{ Z_{i;i} Z_{t+i;i+k} : 1 \leq i < N \} \) can be implemented with circuit of depth 1. Eventually, the depth of Hamiltonian \( H^{QUBO} \) is of order \( \Theta(N) \).

The detailed analysis for each encoding can be found in Supplementary materials.

### Numerical analysis

In order enable the simple reproduction of our results, we publish our code on GitHub [30]. Below we present a detailed explanation of the optimization procedure.

Let us describe the optimization algorithm we used to generate the result presented in Fig. 4. We have emulated the quantum evolution and take an exact expectation energy of the state during the optimization. As a classical subroutine we used a L-BFGS algorithm implemented in Julia’s Optim package [31]. Independently of the in-
We took QUBO and HOBO encodings of TSP with a valid route. Since the energy values for both QUBO and HOBO encodings are incomparable, we decided to present the probability of measuring the feasible solution, i.e. the solution describing a valid route. For objective Hamiltonian we assumed the parameter \( \theta_{obj} \) will be from \([0, R]\). For both we assume periodic domain, mainly if \( \pi + \varepsilon (R + \varepsilon) \) was encountered, the parameter was changed to \( \varepsilon \), which changed the hypercube domain to hypertorus.

Let \( r \) be the level numbers of the circuit. For \( r < 5 \), each run was started from randomly chosen vector within the range of the parameters. For \( r \geq 5 \), we used a trajectories method similar to the one proposed in [32]. First we optimized the algorithm for \( r = 5 \), as described in previous paragraph. Then, for each \( r \geq 5 \) we took the optimized parameter vectors \( \vec{\theta}_{mix}^{(r)} \), \( \vec{\theta}_{obj}^{(r)} \) of length \( r \), and constructed new vectors \( \vec{\theta}_{mix}^{(r+1)} \), \( \vec{\theta}_{obj}^{(r+1)} \) of length \( r + 1 \) by copying the last element at the end. We took these vectors as initial points for \( r + 1 \). Therefore we obtained a trajectory of length 11 (for figure [2]) of locally optimal parameter vectors, one for each \( r \geq 5 \).

Sometimes the algorithm has not converged to the local optimum in reasonable time. We claim that the reason came from periodicity of the domain, which for general TSP breaks the smoothness of the Hamiltonian landscape. We only accepted runs for which: for \( r < 5 \) the gradient was below \( 10^{-5} \); for \( r \geq 5 \), for each parameters vector from the trajectory, the gradient was supposed to be below 10\(^{-5} \).

Since the energy values for both QUBO and HOBO are incomparable, we decided to present the probability of measuring the feasible solution, i.e. the solution describing a valid route.

For estimating the number of measurements we applied the Hoeffding’s inequality. Let \( X = \frac{1}{M} \sum_{i=1}^{M} X_i \) be the mean of i.i.d. random variables such that \( X_i \in [a, b] \). Then

\[
P(|X - \mathbb{E}X| \geq t) \leq 2 \exp \left( -\frac{2M t^2}{b - a} \right).
\]

In our case \( X \) is the energy estimation of the energy samples \( X_i \). Provided that we expect both probability error and estimation error to be constant, we require \( M = \Omega(b - a) \).

The values of \( a, b \) depend not only on the cost matrix \( W \), but also on the form of the encoding and the values of constants \( A_1, A_2, B \) in Eq. (2). For simplicity, we take the following assumptions when estimating the samples number. First, w.l.o.g. we assume \( B = 1 \). Furthermore, we assumed \( C \max_{i\neq j} W_{ij} \leq A_i \leq C^2 \max_{i\neq j} W_{ij} \) where \( C, C^2 \) do not depend on \( N \) and \( W \). This matches the minimal requirement for QUBO. While various measures on \( W \)

| No. of qubits | \( N^2 \) | \( N \log(N) \) | \( 2^{N^2-\alpha} \log N \) | \( N \log(N!) \) |
| No. of terms | \( 2N^3 \) | \( \frac{1}{2} N^4 \) | \( \frac{3}{2} N^{3+\alpha} \) | exponential |
| Circuit depth | \( 12N \) | \( 2N^3 \) | \( 2CN^{1+2\alpha} \) | exponential |
| Circuit volume | \( 12N^3 \) | \( 2N^4 \log N \) | \( 2\alpha N^{3+\alpha} \log N \) | exponential |
| No. of measurements | \( O(N^3) \max_{i\neq j} W_{ij} \) | \( O(N^2) \max_{i\neq j} W_{ij} \) | \( O(N^{3-\alpha} \log N \) max_{i\neq j} W_{ij} \) | \( O(N) \) range(W) |

Table 1: Resources required for various Hamiltonian encodings. Only leading terms are written, for more exact bounds see Supplementary materials. The \( O(\cdot) \) does not depend on the choice of \( W \). We assumed \( B = 1 \) and \( A_1, A_2 \leq O(\max_{i\neq j} W_{ij}) \). Note that \( H_{MIX} \) scales up to logarithmic factor between \( H_{QUBO} \) and \( H_{ROBO} \). For mixed Hamiltonian the constant \( C \) satisfies \( C \in (\frac{1}{2}, 1) \), and in general depends on \( \alpha \) and \( N \).
could be considered, we presented the results in the form $f(N)\max_{t,i}(W)$, where $f$ does not depend on $W$. Furthermore, our analysis for each model is tight in $N$ assuming that $\max_{i\neq j} W_{ij}, \min_{i\neq j} W_{ij} = \Theta(1)$ independently on $N$. Note that using this assumption $a \geq N\min_{i\neq j} W_{ij}$ is valid for any correctly chosen $A_1, A_2$.

Furthermore, Hamiltonians $H_\phi$ and $H_{\text{valid}}$ are integer-valued, and the spectral gap is of constant order. For QUBO, the spectral gap is at most two, which can be generated by adding superfluous one-bit to any valid encoding. For HOBO, it can be generated by choosing the same number for different $b_i, b'_i$. Finally, for the mixed approach we can generate incorrect assignments to slack variables. Theoretically, there is no upper-bound for $A_1, A_2$. However, in general it is not encouraged to make them too large, as classical optimization algorithm may focus too much on pushing the quantum state to feasible state instead of optimizing over feasible space. For this reason and to make the presentation of our results simpler, we assumed that $A_i$ are of order $\max_{i\neq j} W_{i,j}$.

During the optimization, one could expect that the quantum states will finally have large, expectedly $1 - o(1)$ overlap with the feasible space. Thus one could expect that the estimated energy will be of typical, and later close to minimal route. Thus, for these points one could expect that $O(N)\text{range}(W)$ samples would be enough to estimate the energy accurately. We agree that it is a valid approach, especially when the gradient is calculated using $(f(\theta_0 + \varepsilon) - f(\theta_0 - \varepsilon))/(2\varepsilon)$ formula. However, recently a huge and justified effort has been made on analytical gradient estimation, which is calculated based on $\theta$ parameters that are far from the current $\theta_0$ point $\Delta$. In this scenario, we can no longer assume that the energy will be of the order of the typical route. Thus we believe that our approach for number of measurements estimation is justified.

The detailed analysis for each encoding can be found in the Supplementary Materials.

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A Supplementary analysis

A.1 Model resources analysis

In this subsection we will provide a detailed analysis of resources required for each model.

A.1.1 QUBO

Let us recall that the QUBO model takes the form

$$H_{QUBO}(b) = A_1 \sum_{t=1}^{N} \left( 1 - \sum_{i=1}^{N} b_{ti} \right)^2 + A_2 \sum_{i=1}^{N} \left( 1 - \sum_{t=1}^{N} b_{ti} \right)^2 + B \sum_{i,j=1}^{N} W_{ij} \sum_{t=1}^{N} b_{ti} b_{t+1,j}$$

(6)

Number of qubits The model requires $N^2$ qubits.

Number of terms The number of terms can be determined as follows. First we note that we have $N^2$ 1-local terms. Secondly, from the first addend for each $t$ we have $\binom{N}{2}$ 2-local terms, similarly for the second. Finally, for the last part for each $i \neq j$ we have additional $N$ 2-local terms. Note that each 2-local term is present only in one part, which makes our calculation tight. Finally we have

$$\#\text{terms} = N^2 + 1 + 2N \binom{N}{2} + NN(N-1) = 2N^3 - N^2 + 1.$$  (7)

Depth of the circuit Following the reasoning presented in the Method section, we can conclude that the 1-local terms can be implemented with the circuit of depth 1. The first addend from Eq. (6) can be implemented with the circuit of depth $N$ for even $N$, and $N - 1$ for odd $N$, counting $Z_i Z_j$ gates. The second addend can be studied analogously.

For last addend we can independently consider parts $\sum_{i \neq j} W_{ij} b_{ti} b_{t+1,j}$ for even $t$, and then for odd $t$, which will double the circuit depth comparing to fixed $t$. Let us fix $t$. We can implement terms $Z_k = \{Z_i Z_{t+1,i+k}|1 \leq i \leq N\}$ with circuit of depth 1. Since $1 \leq k \leq N$, we can simulate the last addend with the circuit of depth $2N$. Thus in total our circuit has depth $4N + 1$

Since we have $N^2$ qubits, we can simulate at most $N^2/2$ 2-local terms independently. We have $\sim 2N^3$ terms and $N^2$ qubits. The circuit depth for simulating 2-local terms is $\sim 2N^3/(N^2/2) = 4N$, which shows that our analysis is tight.

The calculations were done in terms of gates $\exp(-itZ)$ and $\exp(-itZ_i Z_j)$. Since the latter requires 2 CNOTs and a single rotation gate, we have to triple the circuit depth implementing 2-local gates, which finally gives us $12N + 1$.

Number of measurements For the sake of simplicity we assume that $A_1, A_2 \leq C \max_{i \neq j} W_{ij}$ and $B = 1$. Note that for each $t$, the expression $\left( 1 - \sum_{i=1}^{N} b_{ti} \right)^2$ can be bounded from above by $(N - 1)^2$. We can similarly upperbound the next addend. For the last part we have

$$\sum_{i,j=1}^{N} W_{ij} \sum_{t=1}^{N} b_{ti} b_{t+1,j} \leq N \sum_{i,j=1}^{N} W_{ij} \leq N \binom{N}{2} \max_{i \neq j} W_{ij}.$$  (8)

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Finally we have

\[ H^{\text{QUBO}}(b) \leq A_1 N(N - 1)^2 + A_2 N(N - 1)^2 + BN \left( \binom{N}{2} \right) \max_{i \neq j} W_{ij} \]
\[ \leq CN^3 \max_{i \neq j} W_{ij} + CN^3 \max_{i \neq j} W_{ij} + N^3 \max_{i \neq j} W_{ij} \]
\[ = C' N^3 \max_{i \neq j} W_{ij} \]

Note that the results is tight in order of \( N \), which can be shown using \( b_t \equiv 1 \) assignment.

### A.1.2 HOBO

Let us recall that the model takes the form

\[ H^{\text{HOBO}}(b) = A_3 \sum_{\substack{t=1}}^{N} H^{\text{HOBO}}_{\text{valid}}(b_t) + A_2 \sum_{\substack{t=1 \quad t'=t+1}}^{N} H^{\text{HOBO}}_{\delta}(b_t, b_{t'}) \]
\[ + B \sum_{\substack{i,j=1 \quad i \neq j}}^{N} W_{ij} \sum_{\substack{t=1}}^{N} H^{\text{HOBO}}_{\delta}(b_t, i) H^{\text{HOBO}}_{\delta}(b_{t+1}, j). \]  

Provided that \( \tilde{b}_{K-1} \ldots \tilde{b}_0 \) is a binary representation of \( N - 1 \), we define

\[ H^{\text{HOBO}}_{\text{valid}}(b_t) := \sum_{k^0 \in K_0} b_{t,k^0} \prod_{k=k^0+1}^{K-1} (1 - (b_{t,k} - \tilde{b}_k)^2) \]  
\[ H^{\text{HOBO}}_{\delta}(b_t, b') := H^{\text{HOBO}}_{\delta}(b_t, b') := \prod_{k=1}^{K} (1 - (b_k - b'_k)^2) \]

where \( k^0 \in K_0 \) are such indices that \( \tilde{b}_{k^0} = 0 \).

The proof that \( H^{\text{HOBO}}_{\text{valid}} \) is a valid Hamiltonian for this encoding is presented in Sec. A.2. For the sake of convenience, we will assume \( K = \lceil \log(N) \rceil \), which is at the same time the number of bits in \( b_t \) for any \( t \).

**Number of qubits** The required number of qubits is \( NK + \frac{N}{2} \sim N \log(N) \). The \( \frac{N}{2} \) part comes from the Gray code technique presented in the main text.

**Number of terms** We will assume that \( H^{\text{HOBO}}(b_t, b_{t'}) \) is a Hamiltonian consisting of all terms, meaning that for any factor of this Hamiltonian, the corresponding \( \alpha_S \) is non-zero. While theoretically some terms may vanish, our investigations showed that at least for \( N = 3, 4, 5 \) it is not the case. Furthermore, this guarantees that the bound will be valid for the number of terms in corresponding Ising model.

Due to this assumption, we do not need to consider \( H^{\text{valid}} \) anymore, since terms in \( H^{\text{valid}}(b_t) \) are present in \( H^{\text{HOBO}}(b_t, b_{t+1}) \) as well. For the same reason we do not have to consider elements from \( H^{\text{HOBO}}_{\delta}(b_t, i) H^{\text{HOBO}}_{\delta}(b_{t+1}, j) \).

Note that considering for example \( H^{\text{HOBO}}(b_t, b_{t+1}) \) and \( H^{\text{HOBO}}(b_{t+1}, b_{t+2}) \) we doubly count the terms defined over \( b_t \) only. In general, each term will be counted \( N - 1 \)-times. Taking all of this into account we obtain

\[ \# \text{terms} = \binom{N}{2}2^{2K} - (N - 2)N2^K \leq \frac{1}{2} N^2 2^2 \log N - N(N - 2)2^2 \log N - 1 = \frac{1}{2} N^4 - \frac{1}{2} N^2 (N - 2) = \frac{1}{2} N^4 - \frac{1}{2} N^3 + N^2. \]  

(13)
Depth of the circuit  Similarly as it was done while counting terms, we will only consider implementing $H_{\text{HOBO}}$, as by commutativity $aZ + \beta Z = (a + \beta)Z$.

Following the round-robin schedule we can implement $H_{\text{HOBO}}$ in pairs in at most $N$ steps. Following the Gray code decomposition presented in the main text, we can implement each $H_{\text{HOBO}}$ using a circuit of depth $2 \cdot 2^{2K} - 1$. This gives us a final depth

$$\text{depth} \leq N^2 \cdot 2^{2K} - 1 \leq 2N \cdot 2^{2\log N} - 1 = 2N^3 - 1. \quad (14)$$

Note that factors defined over single $b_t$ will be implemented several times. This conflict can be solved by applying the corresponding angle only once, and for the rest of occurrences applying 0-angle rotation. Since we are not applying rotation in that case, we can reduce the circuit by up to $(N - 1)2^K \approx N^2$, which does not have significant impact on the formula derived above.

It is complicate to reasonable lower bound the circuit’s depth. Since most of the factors are of order $\log N$, one could consider that applying each term requires the depth of the same order as well. However using Gray code ordering it is clear that only two qubits may be needed for applying higher-local terms. For this reason we will assume that at each step only two qubits are required to implement each term. This gives us the lower bound $\approx \frac{1}{2} N^4/(N \log(N)) = \frac{1}{2} N^3/ \log N$ which shows that our approach is tight up to $\log(N)$ factor.

Number of measurements  For simplicity, we will assume that $A_1, A_2 \leq C \max_{i \neq j} W_{ij}$ and $B = 1$. Note that $H_{\text{valid}}$ is a sum of at most $K - 1$ elements, each giving the value either 0 or 1. Hence, for each $t$ we have $H_{\text{valid}}(b_t) \leq K - 1$.

Note that $H_{\text{HOBO}} \equiv H_{\text{HOBO}}$ and $H_{\text{HOBO}}(\cdot, \cdot) \in \{0, 1\}$. Furthermore, since $b_t$ can decode a single number only, $H_{\text{HOBO}}(b_t, i) = 1$ only for a single $i$. Thus

$$\sum_{i,j=1}^{N} W_{ij} \sum_{t=1}^{N} H_{\text{HOBO}}(b_t, i)H_{\text{HOBO}}(b_{t+1}, j) = \sum_{t=1}^{N} \sum_{i,j=1}^{N} W_{ij} H_{\text{HOBO}}(b_t, i)H_{\text{HOBO}}(b_{t+1}, j)$$

$$= \sum_{t=1}^{N} W_{b_t, b_{t+1}} \leq N \max_{i \neq j} W_{ij}. \quad (15)$$

and we can upper bound the energy by

$$H_{\text{HOBO}}(b) \leq A_1 N(K - 1) + A_2 \left(\frac{N}{2}\right) + B N \max_{i \neq j} W_{ij}$$

$$\leq CN \log N \max_{i \neq j} W_{ij} + C \frac{N^2}{2} \max_{i \neq j} W_{ij} + N \max_{i \neq j} W_{ij}$$

$$\leq C' N^2 \max_{i \neq j} W_{ij}. \quad (16)$$

One can again shown the tightness of the bound by using $b_{t_1} \equiv 1$.

A.1.3 Mixed approach  The Hamiltonian takes the form

$$H_{\text{MIX}}(b) = A_1 \sum_{t=1}^{N} H_{\text{valid}}(b_t; \xi_t) + A_2 \sum_{t=1}^{N} \sum_{\nu=t+1}^{N} H_{\text{HOBO}}(b_t, b_{\nu})$$

$$+ B \sum_{i,j=1}^{N} W_{ij} \sum_{t=1}^{N} H_{\text{HOBO}}(b_t, i)H_{\text{HOBO}}(b_{t+1}, j), \quad (17)$$
where \( \xi_t \) are slack variables required to implement \( H_{\text{valid}}^{\text{MIX}} \) and

\[
H_{\text{valid}}^{\text{MIX}}(b_t) := \left( - \sum_{l=1}^{L} \sum_{k=0}^{K-1} b_{lk} + 1 + \sum_{i=0}^{[\log(KL)]} 2^i \xi_{t,i} \right)^2 + \sum_{l=1}^{L} \sum_{k=0}^{K-1} b_{lk} \left( \sum_{l' \neq l}^{L} \sum_{k=0}^{K-1} b_{lk} \right)
\]

(18)

\[
H_{\#}^{\text{MIX}}(b_t, b_v) := \sum_{l=1}^{L} \left( \sum_{k=0}^{K-1} \left( b_{lk} + b_{v,l,k} \right) \right) \prod_{k=1}^{K} (1 - (b_{v,l,k} - b_{l,k})^2)
\]

(19)

\[
H_{\alpha}(b_t, t)^{\text{MIX}} := \prod_{k=1}^{K} \left( 1 - (b_{t', t(i), k} - b_{t,k}^k)^2 \right)
\]

(20)

For a general choice of \( \alpha \in (0, 1) \) it is hardly possible that \( \alpha \log N \) will be an integer number. Hence for fixed \( \alpha \) let \( K := [\alpha \log N] \). Note that \( K \sim \alpha \log N \). On the other hand, we will encounter elements of the form \( 2^K \) and \( 2^{2K} \), for which such an equivalence is not always valid, as

\[
2^K = 2^{\alpha \log N} = 2^{\alpha (N - \varepsilon_{\alpha}(N))} = C_{\alpha}(N) N^\alpha,
\]

(21)

where \( C_{\alpha}(N) := 2^{-\varepsilon_{\alpha}(N)} \) depends on the choice of \( \alpha \) and \( N \), but always \( \frac{1}{2} \leq C_{\alpha}(N) \leq 1 \). Similarly

\[
2^{2K} = 2^{2\alpha \log N} = 2^{2\alpha (N - 2\varepsilon_{\alpha}(N))} = C_{2\alpha}^2(N) N^{2\alpha}.
\]

(22)

Furthermore

\[
L := \left\lfloor \frac{N}{2^K - 1} \right\rfloor \sim \left[ \frac{N}{C_{\alpha}(N) N^\alpha} \right] \sim \frac{1}{C_{\alpha}(N)} N^{1-\alpha}
\]

(23)

Note that if \( N \neq (2^K - 1)L \), then we have to add a separate Hamiltonian of the form similar to \( H_{\text{valid}}^{\text{HOBO}} \), as this encoding will not a encode valid city. This does not change the estimations derived in next paragraphs, as

- it does not require additional qubits,
- it does not produce new terms (they are already included in \( H_{\#}^{\text{HOBO}} \)), and by this it does not change the depth of the circuit,
- it has negligible impact on the energy upperbound, since for each \( t \) the mentioned Hamiltonian will increase energy by at most \( K \).

**Number of qubits** The Hamiltonian requires

\[
NKl + \left\lfloor \frac{N}{2} \right\rfloor L + N[\log(KL)] \sim \frac{\alpha}{C_{\alpha}(N)} N^{1-\alpha} \log N + \frac{1}{2C_{\alpha}(N)} N^{1-\alpha} + N \left( 1 + \log \left( \frac{\alpha}{C_{\alpha}(N)} N^{1-\alpha} \log N \right) \right)
\]

\[
= \frac{\alpha}{C_{\alpha}(N)} N^{2-\alpha} \log N + \frac{1}{2C_{\alpha}(N)} N^{2-\alpha} + N \text{poly}(\log(N))
\]

(24)

qubits. The \( \left\lfloor \frac{N}{2} \right\rfloor L \) is required for implementing the scheduling, while \( N[\log(KL)] \) qubits are needed for \( \xi \) variables.
Number of terms Let us start by calculating the terms generated from $H_{\text{MIX}}$. Let us fix a pair of different time points $t, t'$. The Hamiltonian consists of $L$ independent Hamiltonians defined over $b_{t,i}, b_{t',j}$, which consist of $2^{2K}$ elements. As it was in the case of $H_{\text{MIX}}$, we were over-counting terms defined over $b_{t,i}$ only. Taking this into account we have

$$\binom{N}{2}L2^{2K} - NL(N - 2)2^K \sim \frac{C_{\alpha}(N)}{2}N^2N^{1-\alpha}N^{2\alpha} - N^2N^{1-\alpha}N^\alpha = \frac{C_{\alpha}(N)}{2}N^{3+\alpha} - N^3$$

(25) terms.

Note that in the case of $H_{\text{MIX}}^L$, new factors appear for some $i, j$ with $\bar{l}(i) \neq \bar{l}(j)$. They still are Hamiltonians defined over two binary vectors $b_{t,i}, b_{t+1,j}$, each generating $2^{2K}$ terms. Note that if for some $i', j$ we have $\bar{l}(i) = \bar{l}(i')$, then Hamiltonians

$$\prod_{k=1}^{K}(1 - (b_{t,i}(k) - b_{k}))(1 - (b_{t,j}(k) - b_{k}))$$

and

$$\prod_{k=1}^{K}(1 - (b_{t,i'}(k) - b_{k}))(1 - (b_{t,j}(k) - b_{k}))$$

are defined over the same variables, thus we only have to consider terms over different $l$ instead of different $i$. Taking all of this plus over-counted terms into account, we obtain

$$NL(L - 1)2^{2K} - NL(2L - 2)2^K = NL^2(2^{2K} - 2 \cdot 2^K) \sim N^3 - \frac{2}{C_{\alpha}(N)}N^{3-\alpha}.$$ 

(28)

Finally, let us consider $H_{\text{MIX}}^\text{valid}$. Note that the terms produced by the latter addend were already considered. Hence we need to consider the only terms from the first addend. Let $t$ be fixed. The terms defined over $b_{o}$ only were already considered. We have $[\log(KL)]$ 1-local terms $\xi_{t,i}$. We have $KL[\log(KL)]$ 2-local terms of the form $b_{tik}\xi_{t,i}$. Finally, we have $(\frac{[\log(KL)]}{2})$ terms of the form $\xi_{t,i}\xi_{t,j}$. Taking all of this into account, for each $t$ we have

$$[\log(KL)] + KL[\log(KL)] + \left(\frac{[\log(KL)]}{2}\right) \sim (1 - \alpha)\log N + \frac{\alpha(1 - \alpha)}{C_{\alpha}(N)}N^{1-\alpha}\log^2 N + \frac{(1 - \alpha)^2}{2}\log^2(N).$$

(29)

Taking all numbers above we see that

$$\#\text{terms} \sim \frac{C_{\alpha}(N)}{2}N^{3+\alpha}.$$ 

(30)

Depth of the circuit Let us begin with the terms introduced by $H_{\text{MIX}}$. The Hamiltonian can be splitted into Hamiltonians defined over $b_{t,i}, b_{t',i}$. Note that $l$ are always shared, thus for different $l$, the circuits can be implemented independently. For fixed $l$ we can use the same techniques as for $H_{\text{HOBO}}$, which gives us the depth

$$N(2 \cdot 2^{2K} - 1) = 2C_{\alpha}(N)N^{1+2\alpha} - N.$$ 

(31)

Similarly, the terms introduced by $H_{\text{MIX}}^L$ and not considered before are Hamiltonians defined over $b_{t,i}, b_{t+1,i}$ with $l \neq t'$. In this case we can independently implement Hamiltonians first for even $t$, then for odd $t$, which will double the circuit’s depth. For fixed $t$ we can use similar technique of arranging the Hamiltonians as it was for the last addend of $H_{\text{QUBO}}$. This gives us the depth

$$2(L - 1)(2 \cdot 2^{2K} - 1) \sim 4C_{\alpha}(N)N^{1+\alpha}.$$ 

(32)

In the case of $H_{\text{HOBO}}$ and $H_{\text{MIX}}^L$, we have not taken into account the overcounted elements defined over $b_{t,i}$ only. However, at it was in the case of $H_{\text{HOBO}}$, they do not change the leading factor.
Elements from $H^{\text{MIX}}_{\text{valid}}$ can be implemented using a circuit of depth $3(N + \log(KL)) + 1$, since for each $t$, Hamiltonians can be applied independently, and each $\xi_{t,i}$ has to be applied with all $b_t$ and $b_a$. Part $+1$ comes from applying 1-local terms $\xi_{t,i}$.

Taking all of the numbers derived above we finally have obtain $\sim 2C_2^2(N)N^{1+2\alpha}$.

Similarly as it was in the case of $H^{\text{HOBBO}}_\text{valid}$, the minimum depth in case of mixed approach is 
\[
\frac{C_\alpha(N)}{2}N^{3+\alpha}/(\frac{\alpha}{C_\alpha(N)}N^{2-\alpha}\log N) = \frac{C_2^2(N)}{2\alpha}N^{1+2\alpha}/\log N.
\]

**Number of measurements** For the sake simplicity, we will assume that $A_1, A_2 \leq C \max_{i \neq j} W_{ij}$ and $B = 1$. For general $b$ we have
\[
H(b) \leq A_1 N (L K - 1)^2 + A_1 N \cdot L \cdot K \cdot L K + A_2 \left(\frac{N}{2}\right) L \cdot 2K + BN \max_{i \neq j} W_{ij}
\leq (2CNL^2K^2 + CN^2LK + N) \max_{i \neq j} W_{ij}
\sim \left(\frac{2C_\alpha^2}{C_2^2(N)}N^{3-2\alpha}\log^2 N + CN^{3-\alpha}\log N + N\right) \max_{i \neq j} W_{ij}.
\]

By this we conclude that $H(b) = O\left(N^{3-\alpha}\log N\right) \max_{i \neq j} W_{ij}$. Note that the bound is achievable when taking $b_{tk} \equiv 1$.

**A.2 Proof for $H^{\text{HOBBO}}_\text{valid}$**

**Theorem 1.** Let $N > 0$ and $K$ satisfies $2^{K-1} \leq N < 2^K$. Let $b = \tilde{b}_{K-1} \ldots \tilde{b}_1$ is a binary representation of $N - 1$. Let $K_0 \subseteq \{0, \ldots, K - 1\}$ be indices such that $k_0 \in K_0$ iff $\tilde{b}_{k_0} = 0$ Let
\[
H(b) := \sum_{k_0 \in K_0} \tilde{b}_{k_0} \prod_{k = k_0 + 1}^{K-1} (1 - (b_k - \tilde{b}_k)^2)
\]
(34)
and $b = \tilde{b}_{K-1} \ldots \tilde{b}_0$ be a vector of bits encoding some number $n \in \{0, \ldots, 2^K - 1\}$. Then $H(b) \geq 0$, with equality iff $n < N$.

**Proof.** Note that $(1 - (b_k - \tilde{b}_k)^2)$ is nonnegative, hence $H(b) \geq 0$ independently on $b$. Let $n = N - 1$, which means $b = \tilde{b}$. Then
\[
H(\tilde{b}) = \sum_{k_0 \in K_0} \tilde{b}_{k_0} \prod_{k = k_0 + 1}^{K-1} (1 - (\tilde{b}_k - \tilde{b}_k)^2) = \sum_{k_0 \in K_0} 0 \prod_{k = k_0 + 1}^{K-1} (1 - (\tilde{b}_k - \tilde{b}_k)^2) = 0.
\]
(35)

Let $n < N - 1$. Then there exists a unique $k' \in \{0, \ldots, K - 1\} \setminus K_0$ such that for all $k > k'$ we have $b_k = \tilde{b}_k$, $b_{k'} = 0$. In other words, there exists a bit, which for $N - 1$ is one, and for $n$ is $0$. It is the first one starting from most
significant one. Then we have

\[
H(b) = \sum_{k_0 \in K_0} b_{k_0} \prod_{k = k_0+1}^{K-1} (1 - (b_k - \tilde{b}_k)^2)
\]

\[
= \sum_{k_0 \in K_0} b_{k_0} \prod_{k = k_0+1}^{K-1} (1 - (b_k - \tilde{b}_k)^2) + \sum_{k_0 \in K_0} b_{k_0} \prod_{k = k_0+1}^{K-1} (1 - (b_k - \tilde{b}_k)^2)
\]

\[
= \sum_{k_0 \in K_0} \tilde{b}_{k_0} \prod_{k = k_0+1}^{K-1} (1 - (\tilde{b}_k - \tilde{\tilde{b}}_k)^2) + \sum_{k_0 \in K_0} b_{k_0} \prod_{k = k_0+1}^{K-1} (1 - (b_k - \tilde{b}_k)^2)
\]

\[
= \sum_{k_0 \in K_0} 0 \cdot \prod_{k = k_0+1}^{K-1} (1 - (\tilde{b}_k - \tilde{\tilde{b}}_k)^2) + \sum_{k_0 \in K_0} b_{k_0} (1 - (b_{k'} - \tilde{b}_{k'})^2) \prod_{k = k_0+1}^{K-1} (1 - (b_k - \tilde{b}_k)^2)
\]

\[
= 0 + \sum_{k_0 \in K_0} b_{k_0} (1 - (0 - 1)^2) \prod_{k = k_0+1}^{K-1} (1 - (b_k - \tilde{b}_k)^2) = 0.
\]  

Let \( n > N \). Then there exists a unique \( k' \in K_0 \) such that for all \( k > k' \) we have \( b_k = \tilde{b}_k \) and \( b_{k'} = 1 \). In other words, there exists a bit, which for bit from \( N - 1 \) is zero, and for bit from \( n \) is one. It is the first one starting from the most significant one. Then, taking the addend to \( k_0 = k' \) we have

\[
b_{k'} \prod_{k = k'+1}^{K-1} (1 - (b_k - \tilde{b}_k)^2) = 1 \prod_{k = k'+1}^{K-1} (1 - (\tilde{b}_k - \tilde{\tilde{b}}_k)^2) = 1,
\]

which is enough to prove that \( H(b) > 0 \) as each addend is nonnegative. \( \square \)