Multi-Stage Quantum Walk for Constrained Combinatorial Optimization with Equality Constraints

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***Abstract*—Multi-stage quantum walks (MSQW) are a promising near-term quantum algorithm. Although studies on MSQW have recently been cultivated, there is still limited evidence regarding their effectiveness for constrained combinatorial optimization problems (COPs). This study applied methods proposed in previous studies, which restrict the quantum state to a feasible space and are effective for quantum annealing, to MSQW. As a result, we reveal that the proposed method has the potential to efficiently solve constrained COPs compared to penalty-based naive formulations.**

***Index Terms*—continuous-time quantum optimization, constrained combinatorial optimization problems, multi-stage quantum walk, penalty method, XY model**

I. Introduction

Continuous-time quantum optimization algorithms represent promising approaches for solving combinatorial optimization problems (COPs). Quantum annealing [1] is an established algorithm, whose guiding principle is the adiabatic theorem [2]. The adiabatic theorem guarantees the optimal solution at the final time, provided the evolution is sufficiently slow. However, the required annealing time to satisfy the adiabatic condition increases exponentially with the system size for hard instances, making them intractable on hardware with limited execution time. In contrast, previous studies have proposed multi-stage quantum walks (MSQW) as a promising approach that eliminates reliance on the adiabatic theorem. MSQW enhances the performance of QW [3], [4], which obtains high-quality solutions with short execution times with multiple runs, and the studies related to MSQW have been cultivated [5], [6].

Despite the potential of MSQW, the effectiveness for constrained COPs that are essential for real-world applications remains unexplored. For equality-constrained COPs, one approach proposed in earlier studies [7] demonstrated that restricting quantum annealing to a feasible subspace enhances performance compared to the penalty method.

In this study, we investigate MSQW performance for equality-constrained COPs, comparing the penalty method with a constraint-preserving formulation.

II. Method

Using time t, the MSQW Hamiltonian is expressed as

$$\mathcal{H}(t) = \mathcal{H}_{\mathrm{q}} + \Gamma(t)\mathcal{H}_{\mathrm{p}}, \quad 0 \leq t \leq \tau, \tag{1}$$

where $\Gamma(t)$ is the annealing schedule and τ is the execution time. Here, $\mathcal{H}_{\mathrm{p}}$ is an Ising Hamiltonian whose ground state corresponds to the best solution of the COP, and $\mathcal{H}_{\mathrm{q}}$ is a driver Hamiltonian.

The annealing schedule follows a staircase-like schedule:

$$\Gamma(t) = \begin{cases} \gamma_1, & 0 \leq t \leq \frac{1}{n_{\mathrm{step}}}\tau, \\ \gamma_2, & \frac{1}{n_{\mathrm{step}}}\tau < t \leq \frac{2}{n_{\mathrm{step}}}\tau, \\ \cdots & \\ \gamma_{n_{\mathrm{step}}-1}, & \frac{n_{\mathrm{step}}-2}{n_{\mathrm{step}}}\tau < t \leq \frac{n_{\mathrm{step}}-1}{n_{\mathrm{step}}}\tau, \\ \gamma_{n_{\mathrm{step}}} & \frac{n_{\mathrm{step}}-1}{n_{\mathrm{step}}}\tau < t \leq \tau. \end{cases}, \tag{2}$$

where $\gamma_k = (k-1)\Gamma_{\max}/(n_{\mathrm{step}}-1) + \Gamma_{\mathrm{offset}}$, with $\Gamma_{\max}$ and Γ_{offset} as hyperparameters.

We use the graph partitioning problem (GPP) as a benchmark for COPs with equality constraints. The objective function and constraint term are given by

$$\mathcal{H}_{\mathrm{obj}} = \sum_{(i,j)\in E} \frac{1-\sigma_i^z\sigma_j^z}{2}, \quad \mathcal{H}_{\mathrm{cst}} = \left(\sum_{i=1}^{N}\sigma_i^z\right)^2, \tag{3}$$

where E is the edge set of a random graph with edge density $1/2$, and unit weights. We set $N = 8$. σ_i^α denotes α-component of the Pauli operator on site i. We compare two formulations: (i) Penalty method: $\mathcal{H}_{\mathrm{p}} = \mathcal{H}_{\mathrm{obj}} + \mu\mathcal{H}_{\mathrm{cst}}$, where μ is the penalty coefficient. (ii) XY model: $\mathcal{H}_{\mathrm{p}} = \mathcal{H}_{\mathrm{obj}}$, where the XY model is expressed as $\mathcal{H}_{\mathrm{XY}} = -\sum_{i=1}^{N}(\sigma_i^x\sigma_{i+1}^x + \sigma_i^y\sigma_{i+1}^y)$ with periodic boundary conditions.

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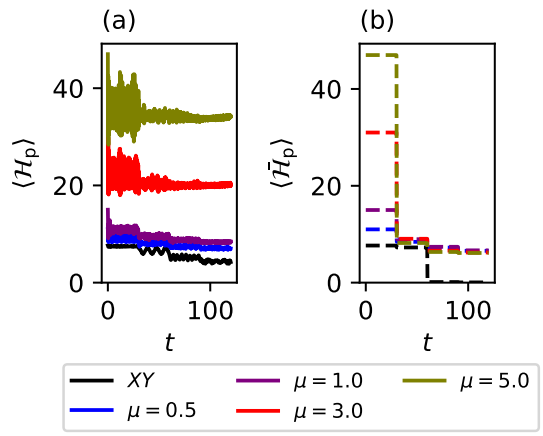

Fig. 1. (a) Dynamics of $\langle \mathcal{H}_\mathrm{p} \rangle$, (b) dynamics of $\langle \bar{\mathcal{H}}_\mathrm{p} \rangle$, for a GPP instance randomly selected from GPP instances with edge density $1/2$ and $N = 8$, and each edge weight is unity. The annealing schedule is determined following Eq. (2) with $\Gamma_\mathrm{max} = 2.0$ and $\Gamma_\mathrm{offset} = 0.5$.

We test penalty coefficients $\mu \in \{0.5, 1.0, 3.0, 5.0\}$ based on the theoretical bounds for homogeneous GPP [8]. We selected the valid parameters to compare the penalty-based naive and constraint-preserving formulations under different conditions by numerically performing MSQW, since the performance of the MSQW depends on the hyperparameters. The number of steps and execution time are set to $n_\mathrm{step} = 4$ and $\tau = 120$, respectively. Also, Γ_offset and Γ_max are set to $\Gamma_\mathrm{offset} = 0.5$ and $\Gamma_\mathrm{max} = 2.0$, respectively. When $\mu = 0.5$, we assume we can theoretically estimate the penalty coefficient. In contrast, when we set larger values of the penalty coefficient, we assume that it is difficult to estimate the penalty coefficient correctly.

For analysis, we decompose the expectation value following [6]:

$$\begin{aligned} \langle \mathcal{H}_\mathrm{p} \rangle &= \langle s | \, e^{\mathrm{i}\mathcal{H}t} \mathcal{H}_\mathrm{p} e^{-\mathrm{i}\mathcal{H}t} \, | s \rangle \\ &= \langle \bar{\mathcal{H}}_\mathrm{p} \rangle + \sum_{E_m \neq E_n} e^{\mathrm{i}(E_m - E_n)t} \langle s | E_m \rangle \langle E_m | \mathcal{H}_\mathrm{p} | E_n \rangle \langle E_n | s \rangle \, , \end{aligned} \tag{4}$$

where $|s\rangle$ denotes the initial state, and E_m and $|E_m\rangle$ represent the mth eigenenergy and eigenstate, respectively. In Eq. (4), $\mathcal{H}$ is the time-independent part of the total Hamiltonian in Eq. (1) during each phase of MSQW in a staircase-like schedule. We refer to $\langle \bar{\mathcal{H}}_\mathrm{p} \rangle$ as the steady-state energy, which reflects the static properties of the MSQW.

III. Result

We investigated MSQW performance by numerically solving the Schrödinger equation via QuTiP [9], [10]. Figure 1(a) shows that expected energy increases with penalty coefficient μ, contrasting with steady-state energy behavior in Fig. 1(b). Large μ values increase the Ising Hamiltonian energy scale, effectively reducing relative annealing schedules and suppressing state transitions, trapping the system in local minima. Small μ values enable better steady-state tracking but may converge to higher steady-state energies. The XY model significantly outperforms the penalty method, achieving both lower expected energies (Fig. 1(a)) and lower steady-state energies (Fig. 1(b)). This demonstrates that the XY model successfully integrates optimal steady-state followability with low steady-state energy by searching only feasible space. Although the hyperparameter conditions that indicate better performance differ in different instances, we also confirmed similar behavior in different GPPs with different system sizes. Therefore, the superiority of constraint-preserving formulation in MSQW will be maintained even in larger system sizes.

IV. Conclusion

The study aimed to evaluate the performance of the MSQW for constrained COPs with equality constraints. The numerical investigation revealed that MSQW with the XY model outperforms MSQW with the penalty method regarding energy dynamics and steady-state energy. This evidence indicates the potential of the MSQW for real-world application with near-term quantum hardware with limited execution time.

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