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Grover search inspired alternating operator ansatz of quantum approximate optimization algorithm for search problems

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Abstract
We use the mapping between two computation frameworks, Adiabatic Grover Search (AGS) and Adiabatic Quantum Computing (AQC), to translate the Grover search algorithm into the AQC regime. We then apply Trotterization on the schedule-dependent Hamiltonian of AGS to obtain the values of variational parameters in the Quantum Approximate Optimization Algorithm (QAOA) framework. The goal is to carry the optimal behavior of Grover search algorithm into the QAOA framework without the iterative machine learning processes.

Keywords Quantum walk · AQC · QAOA · Universal quantum computation · Trotterization

1 Introduction

Quantum technologies have advanced dramatically in recent years, both in theory and experiment. Building a programmable quantum computer involves multiple layers: algorithms, programming languages, quantum compilers, efficient decomposition of unitary operators into elementary gates, the control interface and the physical quantum qubits. The aforementioned requires much research effort for optimization, across and within the layers. From a quantum algorithm perspective, even optimistically assuming the middle layers are perfect, it remains extremely challenging to use quantum algorithms to solve real-life-size hard problems due to size limit and errors arising from

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issues such as precision, random noise and de-coherence in the quantum devices. Hybrid, short shallow circuit algorithms, such as Variational Quantum Eigensolver (VQE) [1] and Quantum Approximate Optimization Algorithm (QAOA) [2], are two near-term answers. From theoretical and implementation aspects, this work aims at investigating two computation frameworks: Grover search and QAOA.

From a perspective of universal computational models, Quantum Walks (QWs) have become a prominent model of quantum computation due to their direct relationship to the physics of the quantum system [3, 4]. It has been shown that the QW computational framework is universal for quantum computation [5, 6], and many algorithms now are presented directly in the quantum walk formulation rather than through a circuit model or other abstracted method [3, 7]. There are multiple quantum computation models, including the quantum circuit model [8–10], topological quantum computation [11], adiabatic quantum computation [12], resonant transition based quantum computation [13] and measurement based quantum computation [14–17]. Notable successes of quantum computation include Shor's factoring algorithm [18] and Grover's search algorithm [19], which manifest indisputable improvements over the best possible classical algorithms designed for the same purpose. QWs can be formulated in discrete-time (DTQW) [20] and continuous-time (CTQW) [3] versions. It is known that Grover search is a special type of DTQW. Since both (QAOA and QW) are universal computational frameworks [5, 6, 21], there should exist some relationship between those models. One can extend the techniques from one framework to another by exploring the connections between the computational models. As the connections are established, one can further investigate if performance-boosting techniques, such as spectral gap amplification [22] and catalyst Hamiltonians [23], can be applied from one framework to the other to provide additional algorithmic improvement.

The structure of this work is as follows. The background on AGS, AQC, QAOA is provided in Sect. 2. The mapping of Grover to AQC is summarized in Sect. 3 and the Trotterization of the schedule dependent AGS to QAOA is given in Sect. 4. We give our the error analysis in Sect. 5. Finally our conclusion is given in Sect. 6.

2 Background

2.1 Adiabatic quantum computing

In the AQC model, H_0 is the initial Hamiltonian, H_f is the final Hamiltonian where the evolution path for the time-dependent Hamiltonian is

$$H(s) = (1-s)H_0 + sH_f, \tag{1}$$

where $0 \leq s \leq 1$ is a schedule function of time t. The schedule is $s = s(t)$ and t goes from 0 to the total run-time T_a. The variable s increases at a slow rate such that the initial ground state evolves and the system state remains as the ground state throughout the adiabatic process. More specifically, the Hamiltonian at time t

$$H(s(t))|\lambda_{k,t}\rangle = \lambda_{k,t}|\lambda_{k,t}\rangle, \tag{2}$$

where $\lambda_{k,t}$ is the corresponding eigenvalue for the k eigenstate $|\lambda_{k,t}\rangle$ at time t. For instance, $|\lambda_{0,t}\rangle$ is the ground state at time t. The minimal eigenvalue gap is defined as

$$g = \min_{0 \le t \le Ta} (\lambda_{1,t} - \lambda_{0,t}), \tag{3}$$

where T_a is the total evolution time of the AQC. It is known that $T_a \propto \frac{1}{g^2}$. Let $|\psi(T_a)\rangle$ be the state of the system at time T_a evolving under the Hamiltonian $H(s(t))$ from the ground state $|\lambda_{0,0}\rangle$ at time $t = 0$. The adiabatic theorem [24, 25] states that the final state $|\psi(T_a)\rangle$ is ϵ_1-close to the real ground state $|\lambda_{0,T_a}\rangle$ as

$$|\langle \lambda_{0,T_a} | \psi(T_a)|^2 \le 1 - \epsilon_1^2, \tag{4}$$

provided that

$$\frac{|\langle \lambda_{1,t} | \frac{dH}{dt} | \lambda_{0,t} \rangle|}{g^2} \le \epsilon_1. \tag{5}$$

2.2 Quantum approximate optimization algorithm

QAOA is a promising approach for programming a near-term gate-based hybrid quantum computer to find good approximate solutions of hard combinatorial problems. In the near future, the number of reliable quantum gates will be limited due to noise, de-coherence and scalability. Due to this fact, hybrid quantum-classical algorithms have been proposed to make the best of available quantum resources and integrate them with classical routines. Technically, QAOA [2] is a variational ansatz that uses p sets of alternating non-commuting (Z-basis associated with parameter γ and then X-basis associated with parameter β) operations on an initial $|+\rangle^{\otimes n}$ state. With each of the p steps, the state evolves with two unitaries,

$$U_t = exp(-i\gamma_t H_c) \text{ and } V_t = exp(-i\beta_t H_0), \tag{6}$$

where H_c is the cost Hamiltonian of the given optimization (or search) problem in the computational basis while $H_0 = \sum_i \sigma_i^x$ with σ_i^x being the Pauli X matrix for the i qubit. In the Noisy Intermediate Scale Quantum (NISQ) computing era [26], it is desirable to use shallow circuits to obtain solutions with high accuracy. Hence, p invocations of the QAOA operator would be

$$U_{qaoa} = \prod_{t=1}^{p} V_t U_t, \tag{7}$$

and p is expected to be some small number to avoid unnecessary decoherence. QAOA aims at solving optimization problems with a short circuit and provides acceptable approximate solutions. Numerous studies have been conducted to find optimal β, γ for each of the step for a shorter circuit and benchmark the performance of QAOA

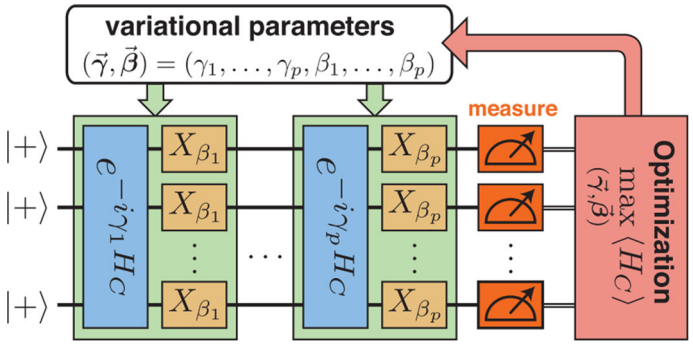

Fig. 1 QAOA with classical optimizer to find the optimal parameters of $\{\gamma_i, \beta_i\}$ as $\{\vec{\gamma}, \vec{\beta}\}$. [31]

[27–30]. In practice, in order to find the optimal values of β_i and γ_i parameters, several iterations of optimization are required as illustrated in Fig. 1 [31]. The final state is measured to obtain expectation value with respect to the objective function H_c. Then the result is fed to the classical optimizer. Based on the condition one sets in the machine learning process, the process for obtaining the variational parameter values for the next iteration stops when no more improvement can be found or the improvement is negligible. However, the post-processing of optimization to find proper values of β_{i+1} and γ_{i+1} from the i iteration using machine learning might be costly.

In the following sections we explore the connection between QAOA and AGS. Here AGS refers to applying the AQC time-dependent Hamiltonian approach to Grover's problem searching for a marked element in the unstructured database. An unstructured search problem of size $N = 2^n$ where the adjacency matrix A has ones everywhere except all zeros on the diagonal. Let $|\omega\rangle$ be the target state while $|s\rangle = |+\rangle^{\otimes n}$ be the initial uniform superposition state. Our initial investigations on the process of mapping CTQW and AGS to QAOA via AQC can be can be viewed as Fig. 2. The Grover inspired approach AGS was first introduced in [32]. There are two paths as shown in Fig. 2, one is CTQW-AQC-QAOA while the other is AGS-AQC-QAOA. This work is mainly for the AGS-AQC-QAOA path. The AGS based path does not cause irreconcilabilities but the CTQW based path did [33]. A more detailed explanation regarding the irreconcilability and potential solutions is at the appendix A for the CTQW-AQC-QAOA path.

3 Mapping: Grover search to AQC

The time-dependent Hamiltonian approach [32] was applied to the Grover's search, searching a marked item in an unstructured database. Grover's algorithm was originally presented as a discrete sequence of unitary logic gates. In [32] it turns to another type of quantum computation where the state of the quantum register evolves continuously under the influence of some driving Hamiltonian. By adjusting the evolution rate of the Hamiltonian so as to keep the evolution adiabatic on each infinitesimal time interval, the total running time is of order $\sqrt{N}$ where N is the number of items in the database.

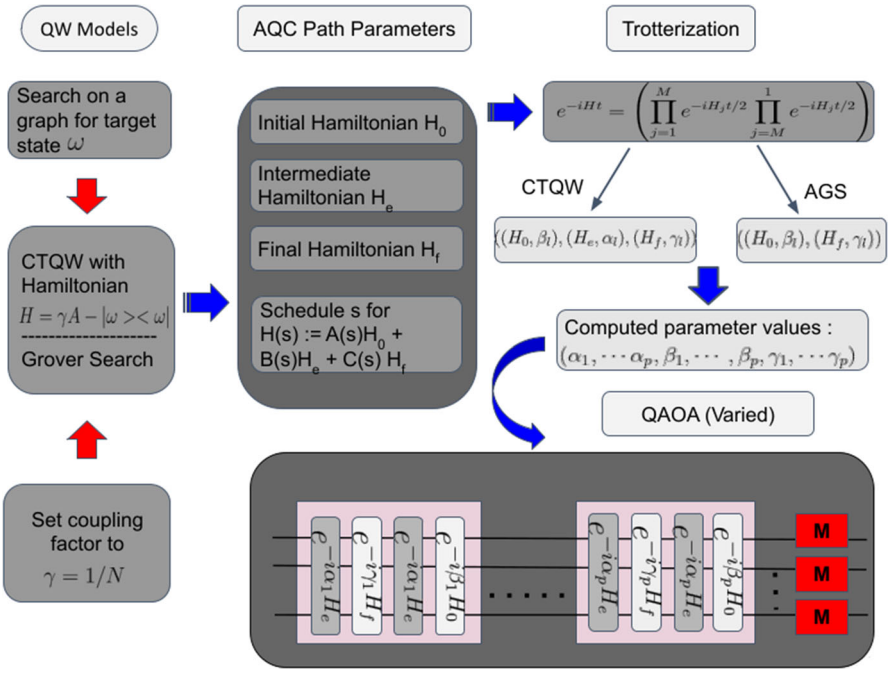

Fig. 2 The process of translation from QW based framework to QAOA to obtain the values of variational parameters in QAOA. One path is CTQW-AQC-QAOA while the other is AGS-AQC-QAOA

Let the time-dependent Hamiltonian as defined in Eq. (1) with the initial Hamiltonian H_0 and the final Hamiltonian H_f being

$$H_0 = I - |\psi_0\rangle\langle\psi_0|, \quad H_f = I - |\omega\rangle\langle\omega|. \tag{8}$$

By such a setting, the initial uniform superposition state $|\psi_0\rangle$ is the ground state for H_0 and the target state $|\omega\rangle$ is the ground state for H_f. The system state evolves in the $\{|\omega\rangle, |r\rangle\}$ basis with the Hamiltonian as [33]

$$H(s) = \begin{pmatrix} (1-s)\frac{N-1}{N} & -(1-s)\frac{\sqrt{N-1}}{N} \\ -(1-s)\frac{\sqrt{N-1}}{N} & 1-(1-s)\frac{N-1}{N} \end{pmatrix}. \tag{9}$$

Following the adiabatic theorem, at any time t during the evolution,

$$\langle -|-\rangle \, E_0(t)'' - \psi_0(t)''^2 \geq 1 - \epsilon_1^2, \tag{10}$$

where $E_0(t)$ is the true ground state and $\psi_0(t)$ is the system state following the adiabatic evolution. Instead of using a linear evolution of $s(t)$, in [32] it adapts the evolution ds/dt to the local adiabaticity condition. It is therefore

$$|\frac{ds}{dt}| = \epsilon_1 g^2(t), \tag{11}$$

where $g(t)$ is the energy gap of the system at time t. The running time t is a function of the interpolation schedule s such that

$$t = \frac{N}{2\epsilon_1\sqrt{N-1}}\Big\{\arctan(\sqrt{N-1}(2s-1)) + \arctan(\sqrt{N-1})\Big\}, \tag{12}$$

and the schedule satisfies the adiabatic theorem. It is further shown that the running time is optimal as $T = O(\sqrt{N})$ when $s = 1$ [32]. By the trigonometry formula $\arctan(x) + \arctan(y) = \arctan\left(\frac{x+y}{1-xy}\right) \bmod \pi$ and the approximation $N \simeq N-1$ when N is large, we know that the angle for the tangent function is bounded as

$$0 \leq \frac{2t\epsilon_1\sqrt{N-1}}{N} \leq \pi \tag{13}$$

which echoes the fact that $0 \leq t \leq T$ when ϵ_1 is some negligible constant. The interpolate schedule s with respect to time t is

$$s = \frac{\sqrt{N}\tan\left(\frac{2t\epsilon_1}{\sqrt{N}}\right)}{2\left(\sqrt{N}\tan\left(\frac{2t\epsilon_1}{\sqrt{N}}\right)+1\right)}. \tag{14}$$

4 Connection: AGS to QAOA via AQC

For simplicity, let us define the time-dependent Hamiltonian $H(s)$ in Eq. (9) as

$$H(s) = A(s)H_0 + C(s)H_f. \tag{15}$$

To reflect Eq. (15) in AGS, one can decompose the evolution operator into some large R steps using Suzuki-Trotter formula, the state evolution of the system is

$$U(T) = exp\left[-i\int_0^T H(t)dt\right]. \tag{16}$$

The Suzuki-Trotter decomposition states $e^{A+B} = \lim_{R\to\infty}(e^{A/R}e^{B/R})^R$ and let us choose $\tau = T/R$. Since the system Hamiltonian evolves based on the schedule s, we can further write

$$\begin{aligned} U(T) &\simeq \prod_{l=1}^{R} exp[-iH(s_l)\tau] \\ &= \prod_{l=1}^{R} exp[-i\big(A(s_l)H_0 + C(s_l)H_f\big)\tau] \end{aligned}$$

$$= \prod_{l=1}^{R} \left(e^{-i\tau A(s_l)H_0/2} e^{-i\tau C(s_l)H_f} e^{-i\tau A(s_l)H_0/2} \right), \tag{17}$$

by using the second order Trotter method where s_l is obtained using Eq. (14)

$$s_l = \frac{\sqrt{N}\tan\left(\frac{\pi l}{R}\right)}{2\left(\sqrt{N}\tan\left(\frac{\pi l}{R}\right)+1\right)}, \tag{18}$$

and $t = \frac{lT}{R}$ and $T \simeq O(\frac{\pi\sqrt{N}}{2\epsilon_1})$. To map to QAOA U_{qaoa} operator with p steps where

$$U_{qaoa} = \prod_{l=1}^{p} V_l U_l = \prod_{l=1}^{p} (e^{-i\beta_l H_0} e^{-i\gamma_l H_f}), \tag{19}$$

one can neglect $e^{-i\tau A(s_1)H_o/2}$ because its action on $|+\rangle^{\otimes N}$ yields only a global phase factor. By matching Eq. (17), one sets $p = R$ and obtains

$$\gamma_{l\in\{1,2,\cdots,R\}} = \tau C(s_l), \tag{20}$$

$$\beta_{l\in\{1,2,\cdots,R-1\}} = \tau(A(s_l) + A(s_{l+1}))/2, \tag{21}$$

$$\beta_R = \tau A(s_R)/2. \tag{22}$$

For AGS, the schedule follows Eq. (1) as

$$A(s) = (1-s), \quad C(s) = s, \tag{23}$$

and we will obtain

$$\gamma_{l\in\{1,2,\cdots,R\}} = \tau s_l, \tag{24}$$

$$\beta_{l\in\{1,2,\cdots,R-1\}} = (\tau/2)\big(2 - (s_l + s_{l+1})\big), \tag{25}$$

$$\beta_R = (\tau/2)(1 - s_R). \tag{26}$$

5 Errors

The approximation error from the translation between models is two-fold: one comes from the AQC simulation error ϵ_1 as indicated in Eq. (4) and the other source of error, ϵ_{2k}, is from the Hamiltonian simulation via Trotterization. Let the approximated unitary be $\tilde{U}$ and the expected total error be bounded from above by ϵ, we have

$$\left\| U - \tilde{U} \right\| = \epsilon_{2k} + \epsilon_1 = \epsilon. \tag{27}$$

Now we need to investigate the value of Trotterization steps R to obey the desired ϵ error in the simulation. For even higher-order, let us denote it as $2k$-th order for $k > 0$,

Table 1 The Hamiltonian simulation error ϵ_{2k} and corresponding discrete-time steps R

Variable	ϵ_{2k}	R
AGS	$O((2t)^{2k+1}/R^{2k})$	$O\left(\sqrt[2k]{\frac{(2t)^{(2k+1)}}{(\epsilon-\epsilon_1)}}\right)$

the formula can be constructed recursively and $U_{2k}(t)$ is of the form [34]

$$\begin{aligned}&[U_{2k-2}(s_k t)]^2 U_{2k-2}((1-4s_k)t)[U_{2k-2}(s_k t)]^2\\&= e^{-iHt} + O((Mt)^{2k+1}/R^{2k}),\end{aligned} \tag{28}$$

where $H = \sum_{j=1}^{M} H_j$ and $s_k = 1/(4 - 4^{1/(2k-1)})$. In general, via the above form, arbitrary high-order formulas can be constructed. But in practice the fourth order $(2k = 4)$ is preferred for most practical problems as the cost from constructing more complex higher-order operators would offset the benefits of Trotterization. To confine the simulation error stated in Eq. (27), we must satisfy the condition that $\epsilon_{2k} \leq \epsilon - \epsilon_1$. This immediately shows that R should be chosen accordingly, as listed in Table 1.

Recalling that AGS has the optimal run-time $O(\sqrt{N})$, we have to set $t = O(\sqrt{N})$. When using Trotterization for Hamiltonian simulation, if ϵ_{2k} is some small constant, we can conclude that at $k = 1$, the required discrete-time step is sub-optimal as $R \simeq O(N^{3/4})$. As k increases, R approaches $O(\sqrt{N})$. In our case for variational variable values based on the second order $(k = 1)$ approximation, the corresponding QAOA should obtain an ϵ-close solution with the sub-optimal running time $R = O(N^{3/4})$.

6 Conclusion and future work

In this work, we explore ways to let QAOA simulate the behavior of optimal search by AGS. The motivation is to find the values of variational parameters from a theoretical approach, instead of heuristic approaches. We discover the values of the variational parameters by letting QAOA simulate AGS via AQC. The AGS obeys the conventional AQC and the mapping is straightforward. Finally, from an error control perspective, to achieve the same degree of accuracy ϵ, both mappings indicate they have the same number of Trotterization steps in the big O notation.

For future investigation, we consider the connection between CTQW and QAOA to be another interesting direction. There are several variations of AQC to improve the performance. The variations are based on modifying the initial Hamiltonian and the final Hamiltonian [23, 35] or adding a catalyst Hamiltonian H_e [23]. The catalyst vanishes at the initial and the final times but is present at intermediate times. For instance, a conventional catalyst assisted AQC is expressed as

$$H(s) = (1-s)H_0 + s(1-s)H_e + sH_f. \tag{29}$$

The form of H_e is important but even a randomly chosen catalyst can help in improving run time [23, 36]. The use of catalyst Hamiltonian also suggests an additional variational parameter α is needed when Totterizing to QAOA as shown in Fig. 2.

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Code Availability Data sharing not applicable to this article as no datasets were generated or analysed during the current study.

Declarations

Conflict of interest This work was supported by the Air Force Research Laboratory Summer Faculty Fellowship Program in year 2020 and 2021 under the guidance of Dr. Alsing. The authors have no relevant financial or non-financial interests to disclose.

Appendix A CTQW-AQC-QAOA Path

A.1 Concern

To construct the time-dependent Hamiltonian $H(t)$, one can use the results from [33] where the AQC search follows the CTQW search on a complete graph. By choosing the coupling factor $\gamma = 1/N$ and letting $|r\rangle$ be the uniform superposition of non-solution states such that

$$|r\rangle = \frac{1}{\sqrt{N-1}} \sum_{i \neq \omega} |i\rangle, \tag{A1}$$

the resulting Hamiltonian [37] for CTQW in the $\{|\omega\rangle, |r\rangle\}$ basis is

$$H = \frac{-1}{N} \begin{pmatrix} N+1 & \sqrt{N-1} \\ \sqrt{N-1} & N-1 \end{pmatrix}. \tag{A2}$$

The system state $|\psi(t)\rangle$ evolution path following the unitary e^{-iHt} is considered as the ground state for the adiabatic path. The time-dependent Hamiltonian $H(t)$ with

$|\psi(t)\rangle$ as ground state is [33]

$$H(s) = \sqrt[4]{\frac{s(1-s)}{4\epsilon_1^2 N}}[(1-s)H_0 + \sqrt{s(1-s)}H_e + sH_f], \tag{A3}$$

where the schedule $s(t) = sin^2(\frac{t}{\sqrt{N}})$. The initial, catalyst, and final Hamiltonians in the $\{|\omega\rangle, |r\rangle\}$ basis are

$$H_0 = \begin{pmatrix} \frac{N-2}{N} & -2\frac{\sqrt{N-1}}{N} \\ -2\frac{\sqrt{N-1}}{N} & -\frac{N-2}{N} \end{pmatrix},$$
$$H_e = \begin{pmatrix} 0 & -2i\sqrt{\frac{N-1}{N}} \\ 2i\sqrt{\frac{N-1}{N}} & 0 \end{pmatrix}, H_f = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}. \tag{A4}$$

The Hamiltonians can be further written as [33]

$$H_0 = |\psi_0^{\perp}\rangle\langle\psi_0^{\perp}| - |\psi_0\rangle\langle\psi_0|, \quad H_f = |r\rangle\langle r| - |\omega\rangle\langle\omega|,$$
$$H_e = 2i\sqrt{\frac{N-1}{N}}(|r\rangle\langle\omega| - |\omega\rangle\langle r|), \tag{A5}$$

where $|\psi_0\rangle$ is the initial uniform superposition state. In comparison to the typical expression in Eq. (1), the intermediate extra Hamiltonian H_e in Eq. (A3) facilitates the driving between $|\omega\rangle$ and $|r\rangle$. However, there exists irreconcilability in the CTQW-inspired AQC path.

In Eqn.(A3), the following parameters were computed during the mapping [33]:

- the scaling factor $\propto \sqrt[4]{\frac{1}{N}}$ of $H(s)$,
- the corresponding catalyst Hamiltonian H_e provides power greater than a typical Yes/No oracle,
- the coefficient function of catalyst Hamiltonian H_e as $\sqrt{s(1-s)}$.

The main concerns arising from Eq. (A3) are twofold. One concern is the factor $\sqrt[4]{\frac{s(1-s)}{4\epsilon_1^2 N}}$ of $H(s)$. The adiabatic theorem [38] states that if we prepare system at time $t = 0$ in its ground state and let it evolve under the Hamiltonian $H(t)$, the system achieve a fidelity of $1 - \epsilon_1$ to the target state, provided that

$$\frac{|\langle\frac{dH}{dt}\rangle_{0,1}|}{g_{min}^2} \leq \epsilon_1, \text{ where } g_{min} = \min_{0\leq t\leq T} E_1(t) - E_0(t). \tag{A6}$$

Here $\langle\frac{dH}{dt}\rangle_{0,1}$ are the matrix elements of dH/dt between the two corresponding eigenstates. $E_0(t)$ and $E_1(t)$ are the ground energy and the first excited energy of the system at time t. Given the $H(s)$ in Eq. (A3), one might conclude that a factor of $O(\sqrt[4]{1/N})$

significantly reduces the required time to achieve $1-\epsilon_1$ precision. This might be misleading as the g_{min} of $H(s)$ also carries that factor.
The second concern is that the catalyst H_e provides power greater than a typical Yes/No oracle as it maps non-solution states to a solution state and a solution state to non-solution states. Provided initially the we start with a superposition state with amplitude of $\sqrt{\frac{N-1}{N}}$, it takes time of $O(1)$ for this catalyst to drive to the solution state from the initial state.

A.2 Strategy

To address the irreconcilability issue, we propose to (1) drop factor $\sqrt[4]{\frac{s(1-s)}{4\epsilon_1^2 N}}$ and (2) modify the catalyst Hamiltonian H_e to be a regular oracle. The form of H_e is important but even a randomly chosen catalyst can help in improving run time [23, 36]. Aiming for being optimal in the translated algorithm without considering other constraints, CTQW-inspired adiabatic path has $H_e = 2\sqrt{\frac{N-1}{N}} iXZ$ in the $\{|\omega\rangle, |r\rangle\}$ basis that provides more power than a standard oracle. To avoid disputes, we will drop the imaginary number i and the X operator. The Z alone behaves as a conventional Yes /No oracle. A slight difference is that since we are in the $\{|\omega\rangle, |r\rangle\}$ basis (not $\{|r\rangle, |\omega\rangle\}$ basis), the Z operator behaves like the conventional oracle with an additional minus sign. Let M be the magnitude scalar equal to $2\sqrt{\frac{N-1}{N}}$ computed from CTQW. The new modified $H_m(s)$ schedule is therefore defined as

$$H_m(s) = (1-s)H_0 + f_z(s)MZ + sH_f, \tag{A7}$$

where $f_z(s)$ is our chosen s-dependent coefficient for catalyst Z. In addition to $f_z(s) = \sqrt{s(1-s)}$ in [33], functions that reach their maximum when $s = 1/2$ would be good candidates for $f_z(s)$. For instance, another good candidate is $f_z(s) = \frac{\sin(s\pi)}{2}$. Because of $0 \leq \sqrt{s(1-s)} \leq 1/2, 0 \leq \sin(s\pi) \leq 1$ as $0 \leq s \leq 1$, one has to use $\frac{1}{2}$ on the sine function is to offset the magnitude M to bound the norm of H_e. Based on the modified schedule, oracle-like catalyst Hamiltonian, one can run the experiment by simulation for CTQW-AQC part using Eq. (A7) and compare the result with the optimal AGS-AQC part using Eq. (9). Our initial investigation indicates the modified CTQW-AQC, bypassing the irreconcilability, remains optimal as the AGS-AQC did.

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