Analog Quantum Approximate Optimization Algorithm

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(Dated: December 15, 2021)

We present an analog version of the quantum approximate optimization algorithm suitable for current quantum annealers. The central idea of this algorithm is to optimize the schedule function, which defines the adiabatic evolution. It is achieved by choosing a suitable parametrization of the schedule function based on interpolation methods for a fixed time. This algorithm provides an approximate result of optimization problems that may be developed during the coherence time of current quantum annealers on their way towards quantum advantage.

I. INTRODUCTION

In nature, the dynamics of several relevant systems can be derived from the solution of an optimization problem. Consequently, the development of efficient optimization algorithms has been a central field for computer science, and naturally, this interest in optimization algorithms also arises in quantum computing. One of the most important approaches for solving optimization problems is by employing quantum annealers, with remarkable advances by D-Wave company [1, 2]. In this paradigm, a quantum system is adiabatically driven from an initial Hamiltonian (at time t = 0), with a ground state that is easy to prepare, to a final Hamiltonian (at time t = T), whose ground state codifies the solution of the optimization problem. If the evolution time (T) is sufficiently large, the adiabatic theorem ensures that after the evolution, the system will be in the ground state of the instantaneous Hamiltonian [3, 4]. This approach has been explored for a large variety of problems, from quantum chemistry [5-7] to quantum finance [8] and machine learning [9, 10]. Nevertheless, the adiabatic evolution demands a large execution time. This time is beyond the coherence time for current quantum annealers, which turns the process incoherent; thus, the possibility of reaching quantum advantage is unclear.

On the other hand, hybrid quantum-classical algorithms have received significant attention during the past few years due to the possibility of being implemented in current noisy intermediate-scale quantum (NISQ) devices. These algorithms are focused on the minimization of a cost function. The cost function is codified in the expectation value of quantum observables, including the Hamiltonian, which is computed by a quantum processor using parametrized quantum states prepared via parametrized quantum gates. Finally, the minimization is obtained by using a classical optimization algorithm over the parameters of the quantum gates. Some examples of these classes of algorithms are the variational quantum algorithms [11–13], the digital quantum approximate optimization algorithm (QAOA) [14, 15], the adaptive random quantum eigensolver [16], and the digitized counterdiabatic QAOA [17] among others. This hybrid approach has been fruitful in different areas, from machine learning to quantum chemistry problems [18–23]. Recently, several works have developed faster versions of the hybrid algorithms or their implementation in another paradigm beyond gate-based computing, such as variational algorithms in measured-based quantum computing, and also some fully-quantum algorithms for optimization problems [24–26].

This work proposes an analog version of QAOA by the suitable parametrization of a stepwise schedule function followed by a classical optimization. This algorithm may be suitable for current quantum annealers, finding optimal protocols for coherent evolution of the annealer quantum processor, exploiting all the potential of such devices.

II. ANALOG QAOA

First of all, an adiabatic algorithm is a time evolution given by the following time-dependent Hamiltonian

$$H(t) = [1 - \lambda(t/T)]H_i + \lambda(t/T)H_f, \qquad (1)$$

where H_i is the initial Hamiltonian with a ground state that is easy to prepare, H_f is the problem Hamiltonian with ground state containing the solution of the optimization problem, T is the total evolution time and $\lambda(x)$ is the schedule function with $\lambda(0) = 0$ and $\lambda(1) = 1$. The time evolution is given by

$$U(t) = e^{-i \int_0^t \{[1 - \lambda(\tau/T)]H_i + \lambda(\tau/T)H_f\} d\tau},$$
 (2)

and if we digitize the time, we obtain

$$U(t) \approx e^{-i\sum_{k=0}^{N} \{[1-\lambda(k\Delta t)]H_i + \lambda(k\Delta t)H_f\}\Delta t},$$
(3)

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where $\Delta t = T/N$. Now, by the use of first order Trotter expansion

$$U(t) \approx \prod_{k=1}^{N} e^{-i\left\{\left[1 - \lambda(k\Delta t/T)\right]\Delta tH_{i} + \lambda(k\Delta t/T)H_{f}\right\}\Delta t}$$
$$\approx \prod_{k=1}^{N} \left(e^{-i\left[1 - \lambda(k\Delta t/T)\right]\Delta tH_{i}}e^{-i\lambda(k\Delta t/T)\Delta tH_{f}}\right).$$
(4)

In quantum annealers, H_i is called the mixer Hamiltonian and has the form $H_i = \sum_j \omega_j \sigma_j^x$, while H_f is diagonal in the computational basis in general.

On the other hand, the digital QAOA algorithm is given by the unitary evolution parametrized by 2N real numbers

$$\mathcal{U}(\vec{\alpha},\vec{\beta}) = \prod_{k=1}^{N} \left(e^{-i\alpha_k H_i} e^{-i\beta_k H_f} \right).$$
(5)

Here, $\vec{\alpha} = \{\alpha_1, \dots, \alpha_N\}$, and $\vec{\beta} = \{\beta_1, \dots, \beta_N\}$ are the parameters to optimize with the cost function given by

$$\langle \phi | \mathcal{U}(\vec{\alpha}, \vec{\beta})^{\dagger} H_f \mathcal{U}(\vec{\alpha}, \vec{\beta}) | \phi \rangle, \tag{6}$$

where $|\phi\rangle$ is the ground state of H_i . From Eqs. (4) and (5), we can see that the digital version of QAOA is basically an optimization of the schedule function $\lambda(x)$ in its digital form.

Now, for the analog QAOA (AQAOA) we propose the time evolution given by a time-dependent Hamiltonian in Eq. (1), but using now an schedule function defined in stepwise manner (see Fig. 1)

$$\lambda_{\vec{p}}(x) = f_k(x); \quad k \frac{\Delta t}{T} = \frac{k}{N} \le x \le (k+1)\frac{\Delta t}{T} = \frac{k+1}{N};$$
 (7)

$$f_k(x) = ax^3 + bx^2 + cx + d; \quad f_k(k/N) = p_k,$$

$$f_k(k + 1/N) = p_{k+1}; \quad (8)$$

and $\vec{p} = \{0, p_1, \dots, p_{N-1}, 1\}$. It means that $\lambda_{\vec{p}}(x)$ is given by a cubic interpolation function of the points $(k/N, p_k)$, with $k = \{0, \dots, N\}$ and $P_0 = 0$ and $P_N = 1$. Therefore, now we have the following unitary evolution

$$U_{\vec{p}}(t) = e^{-i \int_0^t \{[1 - \lambda_{\vec{p}}(\tau/T)]H_i + \lambda_{\vec{p}}(\tau/T)H_f\} d\tau},$$
(9)

and the cost function

$$E(\vec{p}) = \langle G_i | U_{\vec{p}}^{\dagger} H_f U_{\vec{p}} | G_i \rangle.$$
⁽¹⁰⁾

Here, $U_{\vec{p}} \equiv U_{\vec{p}}(t)$, and $|G_i\rangle$ is the ground state of the initial Hamiltonian H_i . We need to mention that H_i and H_f can be the Hamiltonians that quantum annealers can implement currently, where our requirement is only the manipulation of the schedule function in the form of a cubic interpolation function. We note that the total evolution time T plays the role of the circuit depth. In this case, it is independent of the number of parameters to optimize, which is a fundamental difference with the digital QAOA. We also require that this evolution is coherent, such that T needs to be smaller than the coherence time of the quantum annealer.



FIG. 1. Parametrized schedule function $\lambda_{\vec{p}}(x)$. The parameters p_j define the points $(j/N, p_j)$, which are interpolated using a piecewise monotonic cubic interpolation.

In the next section, we will test our AQAOA numerically for a cubic interpolation for different problem Hamiltonians H_f . We need to mention that we do not consider $0 < p_j < 1$. As in the digital version of QAOA, the parameters are completely free and only bound by the experimental setup limitations. Then, this class of interpolation allows that $\lambda_{\vec{p}}(x) > 1$ or $\lambda_{\vec{p}}(x) < 0$. This is not a problem because our method is inspired in the adiabatic evolution but does not follow, in general, an adiabatic path. We highlight that our AQAOA only focuses on minimizing the cost function and does not care about the distance to the adiabatic evolution path. Finally, we request that the interpolation is soft, which means that the second derivative, and also monotonic, which means that the second derivative will not change of sign between two contiguous points.

III. NUMERICAL RESULTS

The performance of our algorithm is calculated using the relative error of the energy obtained by our AQAOA, it means

$$\epsilon_{R} = \left| \frac{\langle G_{i} | U_{\vec{p}}^{\dagger} H_{f} U_{\vec{p}} | G_{i} \rangle - \langle G_{f} | H_{f} | G_{f} \rangle}{\langle G_{f} | H_{f} | G_{f} \rangle} \right|, \qquad (11)$$

where $|G_f\rangle$ is the ground state of the final Hamiltonian H_f . Also, we can consider the fidelity

$$F = |\langle G_f | U_{\vec{p}} | G_i \rangle|^2. \tag{12}$$

Nevertheless, the last could fail as a good performance measure for degenerate ground states because our algorithm only focuses on minimizing the energy and does not care about a specific ground state.

For all our examples, we will use the following initial



FIG. 2. Performance of the AQAOA for the one-qubit case given by Hamiltonian of Eq. (14). The horizontal axis is the total time *T* considered for the algorithm in units of ω^{-1} . We calculate the relative error (a) and the fidelity (b), considering one (blue stars), two (orange stars), four (green stars), and eight (red stars) parameters for the algorithm. The black triangles show the performance using a linear schedule function. Figure (c) shows the schedule function for one (blue line), two (orange line), four (green line) and eight (red line) free parameters (dots) for T = 3.

Hamiltonian

$$H_i = \frac{\omega_i}{2} \sum_{j=1}^n \sigma_x^{(j)}, \qquad (13)$$

where $\sigma_x^{(j)}$, is the *x*-Pauli matrix of the *j*th qubit, ω_i is the initial frequency gap for all the qubits, and *n* is the total number of qubits.

A. One-qubit case

For our first example, we consider the following final Hamiltonian for one qubit

$$H_f = \frac{\omega_f}{2} \sigma_z^{(1)}.$$
 (14)

For simplicity, we consider the same frequency for the initial and final Hamiltonian ($\omega_i = \omega_f$). The performance of our algorithm is collected in Fig. 2a for the relative error ϵ_R , and Fig. 2b for the fidelity. Each point (star) represents the performance of the algorithm for different total algorithmic time *T* and a different number of parameters in the minimization process, namely, one parameter (blue stars), two parameters (orange stars), four parameters (green stars), and eight parameters (red stars). Moreover, we compare the performance of our algorithm with the performance of adiabatic quantum computing using the most common schedule function, i.e., the linear schedule function $\lambda(t) = t/T$ (black triangles). From these two figures, we can see that a time of $T = 4 [\omega_i^{-1}]$ is enough for our algorithm to find the solution of the problem with only two parameters, while the linear function needs approximately double time. On the other hand, the algorithm performance using one parameter for the optimization process follows the same performance as the linear schedule function. If we consider a superconducting flux qubit $\omega_i \sim 2$ [GHz], then for a time $T \sim 2$ [ns], our algorithm produces the correct solution using two parameters for a single qubit Hamiltonian. Finally, Fig. 2c shows optimal schedule functions for one (blue), two (orange), four (green), and eight (red) free parameters. We point out that the end points (0.0) and (1,1) are fixed. The oscillations in the schedule functions mean that we are not following an adiabatic evolution, which is also observed by the fact that we have zones where $\lambda_{\vec{n}}(x) > 1$ and $\lambda_{\vec{n}}(x) < 0$. It implies that the adiabatic theorem does not constrain the time for our final result.

B. Hydrogen Molecule

Our next example is a non-stoquastic Hamiltonian describing a hydrogen molecule [27] with a bond length of 0.2 [Å]

(1) (2)

$$H_f = g_0 \mathbb{I} + g_1 \sigma_z^{(1)} + g_2 \sigma_z^{(2)} + g_3 \sigma_z^{(1)} \sigma_z^{(2)} + g_4 \sigma_y^{(1)} \sigma_y^{(2)} + g_5 \sigma_x^{(1)} \sigma_x^{(2)},$$
(15)
with $g_0 = 2.8489$, $g_1 = 0.5678$, $g_2 = -1.4508$, $g_3 = 0.6799$,
and $g_4 = g_5 = 0.0791$. The performance of our algorithm
is shown in Fig. 3a for the relative error ϵ_R and Fig. 3b for
the fidelity. In this case, we consider the same number of pa-
rameters that in the previous case, and again we compare the
performance of the algorithm with the performance using the
linear schedule function, black triangles in the figure. From
these two figures, we can see that for a time of $T = 8 [\omega_i^{-1}]$ the
AQAOA algorithm can find the solution of the problem with
only two parameters with a fidelity larger than 0.99. In this
case, the performance of the algorithm using only one param-
eter for the optimization process improves the performance of
the linear schedule function, obtaining fidelities over 0.95 for
a time $T = 10 [\omega_i^{-1}]$. If we consider a quantum annealer based
on flux qubits, our algorithm gets the correct solution using
two parameters for $T \sim 4$ [ns]. Finally, Fig. 3c shows optimal
schedule functions for a different number of parameters.

C. Ising and Heisenberg Hamiltonians

Finally, we consider the scaling in the total algorithmic time T for two kinds of nearest-neighbor Hamiltonians. First, we consider the stoquastic Hamiltonian of an Ising chain given by

$$H_f = \frac{1}{2}\omega_f \sum_{k=1}^{N} \sigma_z^{(k)} - J \sum_{k=1}^{N-1} \sigma_z^{(k)} \sigma_z^{(k-1)}, \qquad (16)$$

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FIG. 3. Performance of the AQAOA for the Hydrogen-molecule case given by the Hamiltonian of Eq. (15). The horizontal axis is the total time *T* considered for the algorithm in units of ω^{-1} . We calculate the relative error (a) and the fidelity (b), considering one (blue stars), two (orange stars), four (green stars), and eight (red stars) parameters for the algorithm. The black triangles show the performance using a linear schedule function. Figure (c) shows the schedule function for one (blue line), two (orange line), four (green line) and eight (red line) free parameters (dots) for T = 5.



FIG. 4. Performance of the AQAOA for an Ising chain (blue) and homogeneous Heisenberg chain (orange) with different number of sites. (a) Total running time *T* necessary for fidelity over 0.99 using the same number of parameters as sites in the chain. (b) The relative error ϵ_R for the same cases than in (a).

and second the non-stoquastic Hamiltonian of a homogeneous Heisenberg chain which reads

$$H_{f} = \frac{1}{2} \omega_{f} \sum_{k=1}^{N} \sigma_{z}^{(k)}$$
$$-J \sum_{k=1}^{N-1} \left(\sigma_{x}^{(k)} \sigma_{x}^{(k-1)} + \sigma_{y}^{(k)} \sigma_{y}^{(k-1)} + \sigma_{z}^{(k)} \sigma_{z}^{(k-1)} \right).$$
(17)

For simplicity we consider in both cases $\omega_i = \omega_f = 2J$. We use N parameters for the optimization process for the chain of N sites. This means that if we consider a chain of N = 5sites for the Ising or Heisenberg Hamiltonians, we use 5 parameters in the parametrization of the schedule function. Furthermore, we are interested in the time T needed to get a solution with fidelity over 0.99. These results are collected in Fig. 4a, which shows T for an Ising chain (blue dots) and homogeneous Heisenberg chain (orange dots) as a function of the number of sites N. Moreover, Fig. 4b shows the corresponding relative error ϵ_R for the same cases than in Fig. 4a. We note that for the homogeneous Heisenberg chain, the time T decreases with the number of the qubits in the system. This suggests that with a time $T = 3 [\omega_i^{-1}]$ the algorithm can obtain results with fidelities larger than 0.99 with N parameters for a chain of N sites. On the other hand, the time T for the Ising chain increases with the number of sites and reaches a maximum value in N = 8 sites with a time $T \sim 10 \ [\omega_i^{-1}]$. Finally, in a superconducting circuit platform, an advanced architectures for quantum computing, the frequency ω_i is in the order of a few GHz. It implies that for most superconducting circuit setups $\omega_i > 1$ [GHz] $\Rightarrow \omega_i^{-1} < 1$ [ns], while considering typical coherent times in the scale of microseconds, it means larger than $10^3 \omega_i^{-1}$. Therefore, our AQAOA algorithm gives an interesting approach to achieve fast and high-fidelity approximations for optimization problems suitable for quantum annealers in a coherent manner.

IV. CONCLUSIONS

In this work, we introduced an analog version of the quantum approximate optimization algorithm suitable for current quantum annealers. Our algorithm is based on a general parametrization of the schedule function, which produces any function if we consider enough parameters. By optimizing this parametrization in the same way than in the standard QAOA algorithm, we can coherently produce fast and largefidelity solutions. We test our algorithm numerically for different cases. First, for a single qubit Hamiltonian; second, for the ground state energy of the Hydrogen molecule; and, third, for an Ising and homogeneous Heisenberg chain with different number of sites. The latter ranges from 2 to 10, obtaining in all studied cases high fidelities with a relatively low number of parameters, amounting to the same number of parameters than the qubits in the Hamiltonian.

Furthermore, a possible experimental implementation of our AQAOA depends on two features: first, a quantum annealer capable of producing the desired final or problem Hamiltonian H_f , and, second, a quantum annealer with a schedule function that can be manipulated. The experimental limitations on the final Hamiltonian will determine the classes of problems that we can solve, and depending on the experimental manipulability of the schedule function, our optimization process will require more or fewer constraints.

Finally, this work paves the way for efficient implementations of optimization algorithms in analog devices such as

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current quantum annealers, exploiting the inherent quantum nature of the device.

V. ACKNOWLEDGMENTS

The authors acknowledge support from projects STCSM (2019SHZDZX01-ZX04 and 20DZ2290900), SMAMR (2021-40) and Junta de Andalucía (P20-00617).

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