Addressing hard classical problems with Adiabatically Assisted Variational Quantum Eigensolvers

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We present a hybrid classical-quantum algorithm to solve optimization problems in current quantum computers, whose basic idea is to assist variational quantum eigensolvers (VQE) with adiabatic change of the Hamiltonian. The rational for this new algorithm is to circumvent the problem of facing very small gradients in the classical optimization piece of a VQE, while being able to run in current hardware efficient devices. A discrete concatenation of VQEs adapted to interpolating Hamiltonians provides a method to keep the quantum state always close to a path faithfully directed to find the final solution. We benchmark this Adiabatically Assisted Variational Quantum Eigensolver (AAVQE) on quantum Hamiltonians and hard classical problems, for which our approach shows fast convergence.

I. INTRODUCTION

The success of quantum computation relies on experimental improvements of quantum devices as well as on conceptual progress in the way quantum algorithms are designed. The increasing size of quantum computing prototypes provides enormous challenges to both research fronts. Within the superconducting qubit platform, new ideas to get better gate fidelity, less cross-talk among qubits and the possibility of adding error correction strategies seem to pave a clear avenue for research [1]. It is necessary to match this experimental progress with new ideas on the way quantum computers can be used to solve all sort of problems, both in physics and in real world applications [2].

Quantum algorithms were first developed to produce explicit quantum circuits that solved a task, often related to classical computation. Two of the most relevant instances of this original approach were the algorithms due to Grover [3] and Shor [4]. Both of them exploit the advantage of quantum superposition and parallel processing using quantum circuits. It is, thus, necessary to design specific circuits that take an initial banal quantum state into a final state which encodes the solution to a classical problem. There are not many quantum circuits that serve the purpose to explicitly solve quantum problems. Some exceptions are the ones associated to quantum systems which are integrable [5, 6], and have been verified on actual quantum computers [7]. It is also possible to design a quantum circuit for the Kitaev honeycomb model [8].

A separate class of interest consists of quantum algorithms that solve a task, such as optimization. The original idea of adiabatic quantum computation [3, 10] is a good example. The ground state of a given Hamiltonian can be obtained by first starting from the ground state of a simple Hamiltonian under control. Then the adiabatic theorem states that the two ground states can be connected by evolving with a Hamiltonian that keeps changing in time. To be precise, let us consider a system with $n$ qubits that evolves with the Hamiltonian

$$H(s) = (1-s)H_0 + sH_P,$$  

where the first Hamiltonian can be chosen to have the simple product structure

$$H_0 = \sum_{i=1,...,n} \sigma_i^x,$$  

and $H_P$ is a problem Hamiltonian whose ground state encodes the problem solution. The parameter $s$ can be made to change in time from 0 to 1, that is, $s = s(t/T)$, being $T$ the total running time of the evolution. Given this conditions, the adiabatic theorem states that the initial ground state of $H_0$ will evolve to the ground state of $H_P$, providing the solution to the problem, if the evolution remains slow enough. To be precise, the probability error is given by

$$P(error) = \max_s \left| \frac{\langle \psi_1 | \frac{dH(s)}{ds} | \psi_0 \rangle}{g(s)^2} \right|,$$

where the numerator corresponds to the transition amplitude between the ground state and the first excited state, and the denominator is the gap of the system. The theorem indicates that the source of error is related to the possibility of jumping from the ground state to the first excited state, either because the amplitude for such a process is large or due a very small gap. In this language, hard problems are associated to adiabatic evolutions where the gap becomes exponentially small.

A new category of algorithms has been put forward under the name of Variational Quantum Eigensolvers (VQE) [11, 12]. The basic idea is to consider quantum circuits which can be parametrically constructed from a reduced set of gates. By proper tuning of the
II. THE AAVQE ALGORITHM

Quantum algorithms should bring a quantum system from a state which is easy to prepare to another state which encodes the solution to a problem. An obvious difficulty for any quantum algorithm is how to find a fast and reliable way to connect both states, given the exponential size of the Hilbert space. As mentioned previously, a relevant class of multi-purpose quantum algorithms is the one labeled as VQE. The central idea is to use a parametrized quantum circuit as a provider of variational ansatz to find the ground state of a Hamiltonian. The algorithm proceeds by using a classical characterization of the quantum circuit which is then explored using optimization techniques. The class of VQE is an example of hybrid algorithms that try improve the potential of quantum circuits with classical assistance.

This idea faces the problem of finding a reasonable path in the parameter space of the circuit to end up with the right solution. Notice however that it is possible to strongly argue against this strategy in the following way. Given the exponential size of the Hilbert space, any technique that searches for paths in the parameter space that characterizes the quantum circuit is bound to deal with very tiny gradients. These gradients can even be exponentially small. In such a case, the algorithm may not find the right gradient and would be shooting around in a random way. No convergence to a good result would be seen, specially for large problems.

It is clear that adiabatic evolution gives a guaranteed path to find the ground state of a Hamiltonian, but this procedure may need a very slow evolution. It is also true that VQE may get lost in the search of a minimum. We may summarize the pros and cons of both methods in the following way:

- **Variational Quantum Eigensolver**
  - **PRO:** Uses an arbitrary quantum circuit that is described by a set of parameters to generate variational a ansatz to minimize the problem Hamiltonian.
  - **PRO:** Searches for the gradient in parameter space using classical optimization.
  - **CON:** May get lost in parameter space.
  - **CON:** Uses a large number of measurements.

- **Adiabatic Quantum Evolution**
  - **PRO:** Always finds its way to the solution.
  - **PRO:** Can be optimized to pick a more efficient adiabatic path.
  - **CON:** May be exponentially slow.

The new idea we here put forward is to combine the virtues of adiabatic evolution with those of the VQE strategy. We coin the term Adiabatically Assisted Variational Quantum Eigensolvers (AAVQE) for these class of algorithms. The basic idea is represented in Fig. 1. The algorithm works by applying VQE to a series of Hamiltonians that keep evolving from a simple one to the problem we need to solve.

![FIG. 1: Scheme for the AAVQE algorithm. The Hamiltonian problem is encoded as the end point of a discrete adiabatic interpolation, $H(s) = (1 - s)H_0 + sH_F$, where $s$ takes values between 0 and 1, that is $s = 0, s_1, s_2, \ldots, s_T$ and $s_T = 1$. At each stage of the computation a VQE solves for the ground state of the intermediate Hamiltonians. The arrows represent these classical optimization processes. After minimization at step $s_i$, the characterization of the optimized quantum circuit is used as the initial parameters for the $s_{i+1}$ minimization. The Hamiltonian is then changed and a new VQE is operated.](image)

Let us make the algorithm concrete. We first create a Hamiltonian suited for adiabatic evolution following the form of Eq. 1. This Hamiltonian, though, will never be used for any real time evolution. Instead, we shall consider each discrete step as a new problem to be solved using a VQE. At every step of the computation, the VQE needs the quantum circuit to be initialized with a classical set of parameters $\theta^{(i)}_s$ (initially this set can be chosen randomly). After minimization is complete the quantum circuit is defined by the trained final set of
parameters $\theta^{(f)}_{s_i}$. We then use as initial parameters those obtained in the previous step. This means that the final parameters that deliver the optimal minimum for the Hamiltonian at any step $s_i$ are passed as initial parameters for the next one, that is $\theta^{(f)}_{s_i} = \theta^{(0)}_{s_{i+1}}$.

There are two main differences of our algorithm with respect to the traditional adiabatic evolution, each one serving adiabatic evolution and VQE in both directions. The first one is that no real time evolution is made to get to the next correct ground state. A discretized adiabatic evolution is just used to guide a series of VQEs to find its way to the final Hamiltonian groundstate. The second is that VQE provides a better groundstate to be used at the subsequent step in the adiabatic evolution series. The role of the adiabatic interpolation is simply to guide the series of VQE that deliver a flow of ground states towards the final solution. The summary of the algorithm reads:

1. Prepare the ground state of a simple Hamiltonian with $s_0 = 0$ with a quantum circuit using VQE. Its final characterization is given by the parameters $\theta^{(f)}_{s_0}$.
2. Add a step $\Delta s$, that is $s_{i+1} = s_i + \Delta s$.
3. Run a VQE on $H(s_{i+1})$ using as initial parameters $\theta^{(0)}_{s_{i+1}} = \theta^{(f)}_{s_i}$, the final parameters from the previous step.
4. If $s = 1$ stop, else go to 2).

The combination of adiabatic optimization and variational eigensolvers has been explored before, i.e. Ref.[12] where the particular choice of the adiabatic is the subject of a VQE optimization. The final state preparation improves as a particular path among a parametrization is selected. In the examples presented in our work, this path is fixed. In Ref.[17], an adiabatic strategy is used over the QAOA algorithm[18]. The Trotter parameters are the subject of the optimization, and are evolved following an adiabatic transformation similar to the one presented here. Our work makes no use of a particular Hamiltonian evolution and the quantum circuit employs has no relation to the problem hamiltonian. This leads to the application of the AAVQE to problems without an explicit implementation of the circuit Hamiltonian, such as classical optimization problems, making quantum optimization available to any quantum circuit defined by classical parameters. In the Results section below we show that precisely these problems benefit specially from an adiabatic approach.

There are two main tunable options in the AAVQE algorithm. First, the detailed discretization of the adiabatic change of $H(s)$ is a matter of choice. The more steps we use, the easier will be for the algorithm to remain in the ground state but more calls to the quantum circuit will be needed. The scaling of the running cost of the algorithm is linearly proportional to this discretization. If $s$ is divided in $T$ steps, the number of quantum gates which are needed grows as $T$. It is also possible to look for optimal discretization of adiabatic evolution which are not linear. Second, the classical optimization method used to find the gradient towards the ground state is also a choice in the hands of the programmer. If we consider simple methods based on computations of local gradients, it is then a matter of how this gradient is computed. All in all the algorithm has a good amount of freedom we shall explore in the next chapter.

Let us note that AAVQE works for any kind of final problem, let it be classical or quantum. We shall explore both cases later on. In practice, each VQE needs to minimize a function which is obtained as measurement on the state produced by the circuit. In the case that the minimization function can be read directly from the output probabilities in each qubit in the computational basis, the problem is essentially equivalent to a diagonal Hamiltonian. If, instead, we optimize a Hamiltonian involving many-body operators terms, expectation values of composite operators will form the fit function used by the classical optimization part of the algorithm.

There is a further relevant conceptual advantage for AAVQE over VQE, which is related to the possibility of VQE to get trapped in a local minimum. That is, VQE, being a plain minimization strategy, can converge to a quantum circuit which is not delivering the state with an absolute minimum of energy. Instead, adiabatic evolution may be slow but it will go to the right minimum. This is to be taken with a grain of salt, as adiabatic evolution may end up jumping to an excited state if it runs too fast. Still, adiabatically assisted eigensolvers may have the right balance to avoid local minima, as we shall see in our benchmarking.

### III. RESULTS

In our experiments we simulate a quantum circuit controlled by a classical optimization algorithm. We follow a practical approach based on current technology, using design conditions similar to those available in experimental labs (see [13]). This is reflected both in the quantum circuits we optimize, and in the classical numerical methods currently used.

We simulate the quantum circuit and the classical optimization without any noise effect. Having access to the full wavefunction description we may use a full estimation of the energy, or rather simulate the error introduced by quantum measurements. We apply these techniques to a purely quantum problem, namely the XX spin chain with local field $H = \sum \sigma_x \sigma_x + \lambda \sigma_z$, and also to hard instances of a hard classical combinatorial problem, namely the EXACT COVER problem. As with VQE, the quantum circuit is exactly the same for all problems, the only difference in implementation being the classical evaluation of the objective function.
A. Optimization of quantum problems

Experimental implementations of the VQE method have been successfully applied to Chemical problems [15]. The classical optimization in this setup is performed by the SPSA algorithm [19, 20], which offers an efficient procedure to obtain the ground state of a quantum model using a reduced number of energy evaluations. The method provides an estimate of the gradient function around the evaluation point, and this gradient is used to decide the optimization direction in the following evaluation of the energy.

While the SPSA efficiently solves local problems, the optimization relies solely on geometric properties of the evaluation function. Thus, for some instances it may face problems to determine a valid optimization direction, resulting in local minima. As the evolution of the optimization of the SPSA method tries to fine grain a good solution, escaping the local minima gets harder at final stages of the optimization. We observe convergence to the correct value, some instances fail to converge in the last stages. In this region energy levels for this systems lie closer, so convergence of the method is harder. This can be easily solved running only the last stages using the parameters from the last optimization as an initial point.

The total evolution of the AAVQE algorithm for an XX spin chain with $N = 4$ is shown in Fig. 4. We plot the energy values –as evaluated by the quantum circuit– at each intermediate evolution of the VQE solution, for each $H(s)$. Here we observe the effect of successive changes in $H(s)$, as the initial $\theta^{(0)}_s$ does not correspond to the ground state of the new Hamiltonian, producing an energy pike. This is rapidly corrected by the new optimization, which produces a new ground state for $H(s_{i+1})$. The final ground state encodes the solution to the target problem.
provided directly by the adiabatic theorem. For each $H(s_i)$ we may stop the optimization upon convergence, reducing the numerical effort for easy values of $s_i$. Upon failure to converge, we may restart the optimization at our best solution of a near problem $H(s_i)$, as we may efficiently store each previous solution. It is easy to detect hard regions of the adiabatic transition, as these normally yield different converged values of the energy (see i.e. Fig. 4). On these regions, one may tune the optimization hyperparameters to carefully converge under harder conditions. We have fixed these parameters in our simulations, so one may only expect better results with a fine parameter tuning.

B. Optimization of classical problems

Frustration-free quantum problems similar to the XX spin chain of the previous section show in general good convergence properties. After a few iterations of the VQE algorithm we may already have a good estimation of the ground state energy. The energy landscape seems to be smooth, and the AAVQE benefits showing good convergence far from regions with a closing energy gap. In this section, we test the AAVQE method on a family of hard classical problems. This scenario shows significant differences with the quantum Hamiltonians explored in the previous section, as frustration may play an important role on the solution space, resulting in harder optimization problems.

We choose instances of the classical EXACT COVER problem –an NP-complete problem–, where a collection of sets of variables is evaluated. Each set, formed by 3 binary variables, is evaluated to true whenever a single variable of the set is 1. A valid assignment satisfies this condition for each set of the collection. We select hard instances for our simulations to stress the exploration of the AAVQE. These instances have a single valid assignment, and are hard as the particular choice of clauses requires a full exploration of the combinatorial possibilities.

This problem may be formulated in a Hamiltonian form using the diagonal expression

$$H_{EC} = \sum_{<i,j,k>} (Z_i + Z_j + Z_k - 1)^2$$

(4)

with local operators $Z_i = \frac{1}{2}(\sigma_i - 1)$. A correct assignment of classical values yields a minimal ground state energy $E_0 = 0$. Each set in the EXACT COVER instance translates into a term in the sum in Eq.(4). A non-satisfying assignment will violate a number of terms in the sum, contributing to the final value of the energy. The minimal gap is therefore 1. The optimization of the ground state may face situations where similar states (as measured i.e. by the Hamming distance) may show very different energies, with effects in a local space exploration of the solutions.

We present in Fig. 5 results of the AAVQE on hard instances of the EXACT COVER problem for $N = 4, 8$. We find the correct assignment of variables at the end of the adiabatic transition. To further stress the performance of AAVQE, we obtained the energy after simulating the effect of a finite number of measurements of the quantum state. Even so, the AAVQE delivers a valid assignment of the variables. While during the adiabatic evolution some partial optimizations may deviate from the ground state of $H(s)$ as the energy spectrum may pre. Interestingly, successive steps of the VQE recover the ground state.
We plot the success of detecting the solution using only real measurements on 1000 iterations in Fig. 6 for $N = 16$, for which we normally find the correct solution in less than 100 iterations and $s < 0.1$. Similar results are obtained up to $N = 20$. As overlap probabilities may be exponentially small for large problems, one may still find good approximate solutions as these are also preferred by the stochastic minimization. However, finding those does not provide any information about the correct solution.

The quantum circuit and the parameter set used in these calculations is exactly identical to that used in the previous section for purely quantum problems, showing the flexibility the AAVQE shows for solving optimization problems. For the same instances, we were unable to find a valid set of parameters of the VQE to solve—or even approximate—these problems (for a detailed exploration see Ref. [21]). As further tuning of the parameters may solve this limitation, this additional numerical effort should be considered while evaluating the performance of the VQE method compared to the AAVQE algorithm.

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