

Quantum algorithms for near-term devices

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Abstract. Here we discuss quantum algorithms for the so-called k -local Hamiltonian problem. This is one of the problems that is QMA-complete which, roughly speaking, is the NP-complete analogue for a quantum computer. We discuss exact methods, both classical and quantum, as well as approximate algorithms, more tailored to existing NISQ (noisy, intermediate-scale quantum) devices. We present a roadmap towards building an algorithmic cooling procedure in a NISQ device and we conclude observing some of the challenges that quantum software engineering might encounter in the future.

Keywords: Quantum algorithms, NISQ.

1 Introduction

Quantum computers are devices that are designed to exploit quantum-mechanical effects in order to solve specific tasks much faster than their classical counterparts (1). As originally envisioned by Feynman (2), they are expected to have a large impact in the simulation of large quantum systems. Additionally, Shor's algorithm for efficient prime number factorization (3) further sparked the interest in quantum computation. Until recently, however, an experiment conclusively demonstrating that current quantum devices can, in some sense, go beyond foreseeable classical capabilities, was lacking. Very recently, in (4) this major milestone was met, in an experiment where a 53-qubit chip was reported to sample from a probability distribution that would have been otherwise impossible to sample from classically in a reasonable amount of time. However, quantum computation finds applications beyond, in areas as diverse as cryptography (3), simulation of quantum systems (5), quantum chemistry (6), optimization (7), search (8), equation solving (9) and machine learning (10), (11), (12).

In order to be successfully addressed, not all the above tasks require the same quantity and/or quality of resources. For instance, integer factorization requires a fault-tolerant, fully scalable quantum computing technology with thousands of logical quantum bits (qubits) and universal quantum gates (13) (see also (14)). In addition, logical qubits should ultimately be encoded into several physical qubits in order to enable recursive quantum error correction, which would increase the qubit and gate count several orders of magnitude (15), (16). For instance, quantum chemistry simulations that go beyond classical capabilities could be performed with few hundreds of qubits, but gate counts based on current realistic parameters give estimates of the

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order of 10^{15} - 10^{16} gates (17), (18). Despite recursive layers of quantum error correction should not be, in principle, a problem once a certain gate fidelity threshold is met (19), and despite some technologies (e.g. silicon (20) or superconducting qubits (21)) indeed rapidly approach the fault-tolerance threshold for error correction on single one- and two-qubit gates, the assumption behind recursive quantum error correction, namely, that the error-per-gate is independent of the system size, still poses a major technological challenge.

On the other hand, currently available quantum devices operate in the so-called noisy intermediate-scale quantum (NISQ) (22) regime. They typically consist of a number of qubits that lies slightly above the limit of brute-force classical simulation (23) (around 50), and their operations are too noisy to allow for recursive quantum error correction to be a viable option. Therefore, NISQ devices can be seen as early quantum computers that can maintain coherence only for a small amount of time. Equivalently, they can carry out algorithms with a fixed number of gates ($10^3 - 10^4$), which would roughly be of the order of the inverse of a single gate fidelity.

Whether NISQ devices can already solve some tasks which cannot be addressed purely by classical means was a matter of intense debate. On the theoretical side, it had been shown that shallow-depth quantum circuits pose an advantage over their classical counterparts (24), even in the presence of quantum noise (25). On the experimental side, the recent experiment of Google (4) showed that this separation does exist, although some criticism followed, based on leveraging a secondary storage to extend the power of classical simulation (26) (See also Section 3.1). However, this criticism is likely to be refuted in the near future, with slightly larger quantum NISQ devices, overcoming the secondary storage argument (see also (27)). It is worth noting that this is but a first milestone, since the problem selected to show quantum inimitability (4) does not have any particular use except for, potentially, certified quantum randomness generation (28), and of course showing this separation between classical and quantum devices.

Most of the potential of NISQ devices is expected, not only in the certified randomness generation area (28), but perhaps more importantly, in optimization problems that are intractable with classical computers. Such optimization tasks, e.g. quadratic unconstrained binary optimization (QUBO), arise naturally in diverse areas of industry, but due to their inherent NP-hardness, classical approaches are only capable of giving sub-optimal solutions by means of heuristics. Despite a NISQ device may not yield the global optimum either (these optimization problems are, in their full generality, what is termed QMA-complete, which is, roughly speaking, the equivalent of NP-complete for a quantum computer), it is open whether they can produce better sub-optimal solutions than classical computers can do (29). NISQ devices have naturally attracted a lot of attention due to their potential in optimization problems, where the cost function is classical. This cost function is represented as finding the ground state of a quantum Hamiltonian that is encoded in the computational basis. Algorithms such as the Quantum Approximate Optimization Algorithm (QAOA) (30) constitute a promising avenue for the solution of such optimization tasks (31).

In this work, we give an overview of the possible approaches that might be relevant for NISQ devices. In Section 2, we consider the k -local Hamiltonian as a benchmark problem and we discuss its complexity-theory implications. In Section 3, we discuss exact quantum algorithms that work in a fault-tolerant quantum computer, which would solve the problem in a worst-case complexity scenario. In Section 3.1 we discuss existing classical approaches and in Section 3.2 we discuss quantum exact methods. In Section 4 we present approximate approaches to the problem; in particular in Section 4.1 we consider methods based on Variational Quantum Eigensolvers, whereas in Section 4.2 methods based on cooling. In Section 5 we sketch a blueprint for an algorithmic cooling algorithm suited for NISQ devices from a platform-agnostic perspective. We conclude in Section 6.

2 The problem of Hamiltonian ground-state energy estimation and preparation

One of the problems that inspired Feynman’s ideas on Hamiltonian Quantum computation (2) is the k -local Hamiltonian problem, defined by Kitaev in (32). In our work we focus in this problem for the following reasons:

- Unlike the classical complexity class NP, where thousands of NP-complete problems are classified, there are relatively few QMA-complete problems that are known.
- This problem can be viewed as a quantum analogue of MAX- k -SAT (how many Boolean clauses involving at most k variables can be satisfied by an assignment), where Boolean variables would be replaced by qubits, and clauses would be replaced by local Hamiltonians, i.e. constraints on sets of, at most, k qubits.
- This is a problem of natural interest in physics, since many of the Hamiltonians appearing in Nature enjoy this property (33), (34).
- A broad class of optimization problems can be recast into a k -local Hamiltonian problem, such that, if we can prepare the ground state of such a Hamiltonian, then we have succeeded in finding the optimal solution.

Hence, the k -local Hamiltonian is a good problem to be our benchmark, due to the above-mentioned reasons. We therefore consider a quantum system of n r -level subsystems described by a Hamiltonian

$$H = \sum_{i=1}^m H_i , \quad (1)$$

where m depends polynomially on n . We say that H is k -local if each of the H_i acts non-trivially in, at most, k sites. We note that being k -local does not necessarily give any information about the geometrical arrangement of the particles. We also say that H is d -dimensional if the particles are arranged in a d -dimensional lattice and only nearest neighbor interactions are allowed. We observe that d -dimensional systems are 2-local.

Preparing the ground state $|\psi_g\rangle$ of H or even finding its ground state energy $\langle\psi_g|H|\psi_g\rangle$ can result into a very complex task. Indeed, many optimization problems can be recast into the form of Eq. (1), even classical NP-complete problems such as 3-SAT or MAX-CUT, simply by taking H to be diagonal in the computational basis. Approximating the ground state of a quantum Hamiltonian is the paradigmatic example of a QMA-complete problem (35). QMA stands for Quantum Merlin-Arthur and it is the set of decision problems for which, if the answer is affirmative, there exists a polynomial-size quantum proof that is accepted with probability greater than $2/3$ by a quantum verifier in polynomial time and, when the answer is negative, no quantum proof convinces the verifier to accept with probability greater than $1/3$. This holds even in perhaps surprising, apparently simpler, particular instances, such as the Hamiltonian being k -local (for $k = 5$ (32), $k = 3$ (36) and $k = 2$ assuming $P \neq QMA$ (37)), or even in a 1-dimensional case (although with qudits of dimension ≥ 12) (35).

One usually finds several approaches when tackling the optimization problem stemming from Eq. (1), which we here briefly recall: Fully classical methods (Section 3.1), quantum exact methods (Section 3.2) methods inspired by variational quantum eigensolvers (Section 4.1) and algorithmic cooling schemes (Section 4.2).

3 Exact algorithms

3.1 Fully classical methods

It is natural to start considering fully classical methods to simulate a quantum computer. This is the first obvious step when developing, benchmarking and debugging a new quantum algorithm or studying quantum processes. However, fully classical methods are of course limited by the exponential growth of the Hilbert space dimension (where quantum states are represented) with the system size, rendering them impractical for even moderate system sizes. The largest simulations, to the best of our knowledge, that have been performed reach up to 49 qubits, intensively exploiting symmetries of the Hamiltonian (23), (28), (38), (39).

To this end, there are basically two *extremal* algorithms (28). The first one (also known as Schrödinger's algorithm) stores all the amplitudes of the wavefunction in the computational basis and updates these amplitudes for every unitary in the circuit that is applied. Clearly, Schrödinger's algorithm cannot be directly applied beyond a system size given by the available memory in the system. The second algorithm (also known as Feynman's algorithm) exploits Savitch's theorem, to allow one to break this memory barrier, keeping it linear in the number of qubits and gates, however at a much larger exponential cost in runtime (28).

Interestingly, the limitation in memory can be overcome, at the expense of a much higher runtime (see also (4), (26)): As a rule of thumb, every halving of the memory requirements (i.e., every extra qubit) comes at the price of multiplying the runtime of the circuit by its depth (28). Regarding the specific problem of ground state prepara-

tion, direct classical algorithms are based on exact diagonalization of H , power iteration methods (40) or Lanczos-based algorithms (41).

3.2 Quantum exact methods

The main advantage that a quantum computer offers is the ability to simultaneously store and manipulate all the amplitudes of the wavefunction. Exact methods for ground state preparation have been developed and improved since the advent of quantum algorithms. Most of the existing algorithms can be classified within two groups:

- In the first group, we would find those which attempt to project a trial, easy to prepare, state onto the ground state by means of phase estimation (42), (43) or filtering (44), which require an implementation of the Hamiltonian dynamics (45), (46), (47), (48), (49), or those that are based on or power-iteration methods (50), (51), which also require the implementation of certain functions of the Hamiltonian, via e.g. linear combinations of unitaries (46), (52), (53).
- In the second group, one can find those which are based on variants of the adiabatic algorithm (54), (55). These aim at preparing an easy state which is the ground state of a known Hamiltonian H_0 , and slowly turning this Hamiltonian into the one we are interested in, H_I , by continuously transforming H_0 into H_I , for instance, by parameterizing the adiabatic path as $H(s) = (1-s)H_0 + sH_I$.

In (50), a method for ground state preparation and ground energy estimation with a quantum computer with a smaller number of qubits than other approaches. If we denote by N the size of H (i.e., N is exponential in n); $|\phi_0\rangle$ (χ) the overlap (a bound on that) between the initial state of the quantum computation and the ground state of H ; Δ the spectral gap of H (the difference between the first excited state energy and the ground state energy); ε the desired precision of the output state with the ground state of H ; Φ the gate cost to prepare the initial state of the algorithm; and Λ the oracle cost to access an element of H in order to implement the Hamiltonian simulation; then in (50) we showed that one obtains an algorithm for ground state preparation with the following quantum gates and qubits requirements:

Table 1. Qubit and quantum gate count for exact ground state preparation algorithms (50).

Algorithm	Gate count (time complexity)	Number of qubits (memory complexity)
Phase estimation + Amplitude Amplification	$\tilde{O}\left(\frac{\Lambda}{ \phi_0 ^2\Delta\varepsilon} + \frac{\Phi}{ \phi_0 }\right)$	$O\left(\log N + \log\frac{1}{\varepsilon} + \log\frac{1}{\Delta}\right)$
Filtering method (44)	$\tilde{O}\left(\frac{\Lambda}{ \phi_0 \Delta} + \frac{\Phi}{ \phi_0 }\right)$	$O\left(\log N + \log\frac{1}{\varepsilon} + \frac{\log\frac{1}{\chi\varepsilon}}{\log\log\frac{1}{\chi\varepsilon}}\log\frac{1}{\Delta}\right)$
(50) with known ground energy	$\tilde{O}\left(\frac{\Lambda}{ \phi_0 \Delta} + \frac{\Phi}{ \phi_0 }\right)$	$O\left(\log N + \log\log\frac{1}{\varepsilon} + \log\frac{1}{\Delta}\right)$
(50) with unknown ground energy	$\tilde{O}\left(\frac{\Lambda}{\chi\Delta^{3/2}} + \frac{\Phi}{\chi\Delta^{1/2}}\right)$	$O\left(\log N + \log\log\frac{1}{\varepsilon} + \log\frac{1}{\Delta}\right)$

Note that in Table 1 the \tilde{O} notation indicates that logarithmic factors have been omitted in the interest of simplicity.

4 Approximate algorithms

From Table 1 we learn that the worst-case complexities deem the problem intractable in its full generality: The parameters $|\phi_0|$ (χ) and Δ are going to be, in general, exponentially small. This should not be surprising, since the k -local Hamiltonian problem is QMA-complete in its full generality. Nevertheless, these are asymptotic results, and they do not imply that NISQ devices may yield an advantage still for low number of qubits. Therefore, our goal in this section is not to exactly prepare the ground state $|\psi_g\rangle$ of H in a worst-case scenario, but to prepare a low-energy state $|\psi\rangle$ within the NISQ framework, ideally achieving a good overlap $|\langle\psi_g|\psi\rangle|$ in an average-case, and benchmark the performance of the algorithm we propose. This means that the set of available quantum gates is limited (given e.g., by the available experimental setup) and the coherence time is upper bounded, thus not allowing for a quantum circuit composed of more than $10^3 - 10^4$ of such quantum gates. In addition, the fidelity of quantum gates would not be good enough to enable fault-tolerant recursive quantum error correction (38), (56), (57).

Our vision is that a shallow quantum circuit that *cheaply* (i.e., with as few operations as possible) boosts the overlap with the ground state $|\langle\psi_g|\psi\rangle|$ allows for much faster quantum exact methods for ground state preparation, as the best dependence with such overlap scales, to the best of our knowledge, as $|\langle\psi_g|\psi_0\rangle|^{-1}$ (44), (50) (see also Table 1). Therefore, in practice, one might be interested in using such a hybrid heuristic-exact approach, even when a scalable, fully fault-tolerant quantum computer would be available.

4.1 Methods inspired on Variational Quantum Eigensolvers

Methods based on variational quantum eigensolvers (VQE) aim at preparing the lowest energy state of H within a parameterized family of wavefunctions. Recently, these methods have gained increasing attention (58), (59), (60), (61), (62), (63). The success of VQE critically depends on the parameterization being general enough, meaning that it should be able to, at least, represent quantum states having high fidelity with the actual ground state but, at the same time, efficient enough, meaning that it should do so with a manageable number of parameters. Tensor network states, such as matrix product states (64), (65), (66), (67), (68), (69) or projected entangled pairs states (70), but also neural quantum states (71), (72), (73), (74) have been shown to successfully represent ground states of physically relevant Hamiltonians. Despite the success of such variational classes of states, except in some cases (63), (75), it is in general not obvious how to prepare such states within the NISQ paradigm.

Interestingly, the so-called Quantum Approximate Optimization Algorithm (QAOA) is specially tailored to shallow-depth devices (30), provided one can perform Hamil-

tonian evolution efficiently. This includes the case of classical optimization problems, when the Hamiltonian terms commute as they are diagonal in the computational basis. Within the NISQ paradigm a classical-quantum continuous feedback loop is normally a key ingredient in the development of such algorithms (76).

4.2 Algorithmic cooling schemes

Schemes based on algorithmic quantum cooling (77), (78), (79), (80) are built upon using ancillary qubits to cool the system of interest: These ancillary qubits weakly interact with the system and are measured after some time. When they are found in an excited state, this process removes energy in the rest of the system. Repeating this process in cycles, produces a monotonically decreasing function of the energy with time, thus achieving the cooling. It is worth mentioning there also exist related, albeit different, approaches based on dissipative open-system dynamics to drive quantum systems to their ground state (81), (82), (83).

5 A blueprint for energy minimization with NISQ devices

In this section, we sketch a blueprint to construct a quantum circuit that heuristically minimizes the energy of a quantum Hamiltonian H . The algorithm is based on an adaptive algorithmic cooling procedure, aided by some classical optimization. Its goal is to approximate a low-energy state of that Hamiltonian with a small number of gates, no extra qubits and few measurements. The method is agnostic to previous insight about the physical properties of the model to be solved, although we benchmark it with 1D systems or exactly diagonalizable models, to show its performance beyond 50 qubits.

Our work incorporates features of the algorithms presented in Sections 4.1 and 4.2 with the vision of being also eventually applicable to improve exact algorithms from Section 3.2 in the future: Indeed, we propose a quantum circuit layout which encodes the variational parameters and we perform the optimization/cooling in a way that the energy is monotonically decreasing at every step. We remark our procedure would still be of interest for a future universal, scalable, fault-tolerant, quantum computer, as it would give a good initial state candidate for the latter application of the exact algorithms in Section 3.2, reducing their necessary runtime.

In our work we do not assume that one can perform any arbitrary unitary per gate, but simply considers the set of interactions that are engineerable in a specific quantum platform. The method we give can be therefore tailored to the experimental possibilities that are available, which greatly vary depending on the physical implementation. By time-evolving an initial quantum state with an interaction h that is available in the lab, we can produce a time-dependent state $|\psi(t)\rangle = e^{-i h t} |\psi_0\rangle$ that will vary the energy of the quantum state as a function of time. By looking at an infinitesimal time evolution, as long as $i\langle [h, H] \rangle \neq 0$, the sign of the previous quantity will tell us whether evolving by $\pm \delta t$ shall decrease the energy. Going to second order, one can then decrease the energy by a non-negligible amount in a single gate.

By exploiting the property that the energy is a monotonically decreasing function with the number of gates, one can build an algorithm that starts with an empty circuit and, from scratch, builds a quantum circuit to decrease the energy of the initial state, eventually converging to a low energy state of H , potentially with a good overlap with the ground state. This algorithm shall be further developed and studied in depth in a future work.

6 Conclusions

This is an exciting time for quantum technologies. The first prototypes of NISQ devices have been developed and, in some aspects, they are starting to go beyond the limits of classical devices. Although the algorithms presented in Section 3 may be out of reach still for some time, those in Sections 4 and 5 are starting to become a reality. This is an intensive, novel field of research, where new algorithms, platforms and experiments appear every day (84), (85), (76), (29), (61), (5), (86), (87), (57), (88), (63).

Here we have presented several approaches to the textbook problem of the k -local Hamiltonian. We have discussed exact methods, approximate solutions and heuristic algorithms to tackle it. We have also seen that it is likely that hybrid approaches will be necessary in the future.

In our case, the vast variety of existing experimental platforms made it non-optional for us to design our algorithm in a platform-agnostic way. The algorithm presented in Section 5 can be further tailored to specific experimental platforms, e.g. where connectivity is limited or only a subset of operations is available. This is but an example of one of the many future challenges that complex, large-scale quantum algorithms might face. As we start to build bigger and more complex quantum systems, the need for the development of a set of good practices to systematically design, implement, test, and document quantum software (i.e., a quantum analogous to software engineering) is likely to become a necessity.

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