Viewing Vanilla Quantum Annealing Through Spin Glasses

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Abstract.
Quantum annealing promises to solve complex combinatorial optimization problems faster than current transistor-based computer technologies. Although to date only one commercially-available quantum annealer is procurable, one can already start to map out the application scope of these novel optimization machines. These mid-scale programmable analog special-purpose devices could, potentially, revolutionize optimization. However, their disruptive application domain remains to be found. While the commercial analog quantum optimization machine by D-Wave Systems Inc. already exceeds 1000 qubits, here it is argued that maybe smaller devices with better quality qubits, higher connectivity, and more tunability might be better suited to answer if quantum annealing will ever truly outperform specialized silicon technology combined with efficient heuristics for optimization and sampling applications.

"The more you know, the more you can create. There's no end to imagination in the kitchen." — Julia Child

Discussing the medium-term impact of current quantum computing devices is a nontrivial task given the different possible implementations. In this brief article some *food for thought* on this subject is presented. It is noted that the expressed opinions are those of the author alone.

1. Amuse bouche — Setting the stage

What can we do with approximately 1000 qubits? That depends strongly on the *kind* of qubits. There are different approaches to using quantum mechanics in computation and, as the reader will notice, the term *quantum computing* [1] is used very carefully within this context. While the ultimate goal is to one day build a digital programmable (universal) quantum computer that fully exploits all the benefits of quantum entanglement and parallelism using 1000 qubits, to date, we are far from this goal. Multiple institutions—either academic, industrial, or governmental—have recently invested heavily in quantum technologies. Small-scale few-qubit programmable devices, such as IBM's publicly accessible superconducting transmon device [2, 3] or a fully-connected five-qubit ion trap device, [4] have been successfully used for computations. However, their scope remains limited due to short coherence times and a small number of qubits. Large corporations, such as Google, IBM, Intel, NTT, and Microsoft, as well as smaller startups such as Rigetti Computing have set ambitious goals [5], however, it remains to be seen how useful their devices will be in the near term.

History has shown that large digital computing revolutions are often preceded by analog developments. The most paradigmatic example being semi-programmable analog vacuum tube computing machines heralding the development of programmable digital transistor technologies. In the quantum computing world, analog semi-programmable quantum optimization machines, such as those manufactured by D-Wave Systems Inc., will likely be remembered as the precursor of programmable digital quantum devices. Like vacuum tubes, or any other analog computing platform, their application scope is limited, because they are designed with a particular purpose in mind — in this case, the minimization of the cost function (Hamiltonian) of a binary (Boolean) optimization problem [6, 7, 8]. This does not immediately imply that quantum annealing machines are doomed to eventually disappear completely. To date, analog silicon devices are used as special-purpose machines in many applications and will likely experience a renaissance as co-processors now that Moore's Law [9] is apparently slowly coming to an end. Furthermore, the development of (analog) quantum optimization co-processors might find applications across different areas of computing, ranging from optimization to machine learning; time will tell.

D-Wave Systems Inc. [10] has pioneered the use of superconducting flux qubits to build semi-programmable analog optimization machines using transverse-field quantum annealing [11, 12, 13, 14, 15, 16, 17]. Quantum annealing, the quantum counterpart of thermal simulated annealing [18] is a sequential optimization technique where quantum fluctuations induced by a transverse field [15, 17] are slowly quenched following an annealing protocol, in the hope of minimizing the cost function of a quadratic binary optimization problem. Although the performance of the device remains controversial to date (see, for example, Refs. [10, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31]), having direct access to the device has advanced quantum computing substantially, as well as revolutionized how we think of optimization today.

In this overview the focus will be placed on *quantum optimization* and *quantum sampling* of cost functions of binary optimization problems. While this scope might seem narrow at first, it is likely that quantum annealing machines will play a central role in the field of quantum optimization (and, more indirectly, in quantum computing) for the next decade. Furthermore, optimization is ubiquitous in scientific, as well as industrial applications. A plethora of optimization problems can be mapped directly onto quadratic binary optimization problems [32]—which are the type of problem current quantum annealing machines are designed to tackle— and so despite its seemingly narrow scope, quantum optimization has the potential to revolutionize machine learning, drug discovery, and industrial distribution, to name a few.

The title of this overview cheekily provides a "view of vanilla quantum annealing through spin glasses." First, *vanilla* quantum annealing refers to the implementation using a transverse field driver Hamiltonian to minimize 2-local cost functions, as it is done in the latest version of the D-Wave Systems Inc. D-Wave 2000Q quantum annealer. More complex drivers could be used with potentially much better performance. Among these could be non-stoquastic driver Hamiltonians with 2-local or even 4-local symmetry. Similarly, multi-qubit native interactions in the problem Hamiltonian beyond quadratic (2-local) would be desirable for many applications. However, these devices remain to be built. Second, spin glasses [33, 34, 35, 36, 37] are likely the hardest simple [38] binary optimization problem. As such, they are perfectly suited for benchmarking any new computing paradigm aimed at minimizing a binary quadratic cost function. Not only are they well understood, but a wide class of optimization problems can be mapped directly onto spin-glass-like Hamiltonian [32]. Multiple recent studies that attempt to gain a deeper understanding of, e.g., the D-Wave device have used variations of spin-glass Hamiltonians. Carefully-designed Ising spin-glass problems can be used

to probe the existence of any quantum advantage (see, for example, Refs. [39, 24, 30, 28]), the effects of noise [40] and chaos [41, 26], the effects of the underlying connectivity on the benchmarking [42, 21], as well as intrinsic limitations of transverse-field quantum annealing, such as poor performance in fair sampling applications [43, 44].

Using the aforementioned approaches in the next sections, it is argued that a large number of qubits is merely an engineering feat and does not necessarily mirror a disruptive quantum optimization device. To build a potentially disruptive device, other equally important metrics should be considered. In what follows, the importance of these other metrics is discussed.

2. Appetizer — The dream annealer

Ideally, special-purpose hardware should be built with an application in mind. This means a highly-optimized bespoke design aimed at solving a particular problem. As such, the "wish list" of features a particular device should have strongly depends on the application in mind. However, if one may imagine a "dream" annealer, such device should have the following properties:

Connectivity – Ideally an all-to-all connectivity is desirable, because there would be no embedding overhead [45]. However, this is a complex task to achieve. At the moment, connectivity is sparse [42]. This means that multiple *physical* qubits have to be used to generate *logical* variables and/or couplers when the problem of interest has an underlying graph that differs substantially from the annealer's hardware graph. As an example, a sparse system with a fixed connectivity like in the D-Wave 2000Q device typically requires $\sim N^2$ physical qubits to generate approximately N fully-connected logical variables [46]. Recent experiments on circuit fault diagnosis problems [47] suggest that a high connectivity might be key in improving the performance of quantum annealing machines.

Coupler order – At the moment, quantum annealers only permit up to two-body qubit interactions. This means that only linear biases that couple directly to individual qubits or qubit-qubit interactions are possible. However, what if the problem of interest has higher-order qubit-qubit interactions? As an example take 3-SAT [48, 49, 50, 51] where each clause has three variables. A Hamiltonian representation of the optimization problem is ideally done with three-way couplers between the Boolean variables. On hardware with two-way couplers, each clause would have to be decomposed, thus requiring more physical variables. A native three-way qubit term in a quantum annealer would require far less physical qubits. Because most problems of interest can be represented as combinations of two-way, three-way and four-way couplers, the dream annealer should have these higher-order couplers. However, recent experiments on circuit

fault diagnosis [47] suggest that higher-order couplers might only show an advantage if paired with more complex driving Hamiltonians.

Better control over noise – Quantum annealers currently are analog devices. Theoretically one can show that [40] to first approximation a doubling of the number of variables should be paired with a reduction of the analog coupler noise by a factor of approximately four. This means that for ever-growing devices, a better control over the hardware and noise sources is needed to be able to encode problems with high enough precision. In fact, many problems of interest, such as the knapsack problem [32], require precision that is currently unattainable in analog quantum annealers.

Better driving Hamiltonians – Although this article focuses on *current* hardware with transverse-field driving Hamiltonians, it would be desirable to have higher-order non-stoquastic drivers to induce more transitions between states and therefore potentially better overcome barriers in the energy landscape. Recent experimental studies have shown (see Ref. [44] and references therein) that transverse-field quantum annealing is a biased sampling approach [43]. The inclusion of more complex drivers might not completely solve the sampling problem, but hopefully improve the overall fair sampling of states.

Error correction – Ideally, quantum error correction should be part of any new quantum annealing machine design, especially because of the inherent analog noise, as well as promising performance improvements observed in previous studies [52, 53]. At the moment error-correction schemes need to be embedded in quantum annealing hardware, thus drastically reducing the number of available variables. Furthermore, typically the native connectivity of the hardware is reduced, thus making the embedding of applications onto the error-corrected system harder. Given these limiting factors, the design of novel quantum annealing hardware should have a built-in error correction component via, e.g., ancilla qubits.

The fabrication of the aforementioned dream annealer with the required specs is unlikely in the foreseeable future. While building a device around a particular application could result in a disruptive quantum optimization device, such application (discussed below) remains to be found. Even worse, it is unclear how to theoretically predict if a particular optimization problem could even benefit from quantum optimization. Given this conundrum, in an effort to not place all eggs in one basket, the construction of quantum annealing hardware has focused on *generic* graphs with simple drivers and two-body interactions between the qubits.

What could one do with a dream annealer and would it be better than current CMOS technology paired with state-of-the-art optimization algorithms? That is unfortunately unclear. In fact, there is no strong evidence to date, that quantum annealing can excel for

any application problem beyond synthetic benchmark problems [54]. And even for the latter the observed speedup does not warrant the effort. So how should the quantum annealing community proceed?

First, determine if quantum annealing can truly deliver an advantage over classical technologies. This could either happen via theoretical studies (desired, as long as realistic hardware considerations are taken into account) or by the development of a (small?) *high-quality* experimental test bed. An example for the former is a theoretical study by Nishimori and Takada [55] where the effects of non-stoquastic terms in the driver Hamiltonian are studied for different optimization problems. While the examples in that work are not realistic, they do highlight the importance of analyzing a problem before implementing it in hardware. In the case of the latter, the IARPA-funded Quantum Enhanced Optimization Program has the goal of addressing if quantum annealing has the potential to outperform classical approaches provided the qubits are of the best quality currently accessible from an engineering standpoint. Small test beds should ideally include the following: First, better control over the qubits than currently available on commercial D-Wave devices. The inclusion of more complex drivers could help elucidate if going beyond transverse fields has potential for quantum speedup and/or better sampling. Having quantum annealers with k-local ($k > 2$) topologies would help in the understanding of the effects of embedding. A similar argument can be made for higher connectivity. Finally, precision far beyond the currently-available 6 bits, (e.g., 32 bits) would open the doors for experimental studies on problems where high precision is key, such as the knapsack problem. This, in turn, could assist in finding an elusive killer application.

Second, develop the necessary know-how to assess the *"quantum potential"* of a given application. The dissection of problems to analyze their potential for a given class of solver/algorithm remains in its infancy. The goal is to measure different metrics that characterize a particular problem and determine its suitability for (in this case) quantum architectures. Simple examples are the embedding overhead or precision requirements. However, there could be far more subtle metrics, such as, for example, measurements that correlate with the shape of the cost function landscape. Fortunately, there is an emergent industry of companies that specialize in bridging the gap between quantum hardware and industrial customers, such as 1QB Information Technologies, Cambridge Quantum Computing, QC Ware, and QxBranch.

Not only is it important to understand which applications work for quantum technologies best, it is as important to also develop sound benchmarking strategies for quantum technologies – the subject of the next section.

3. Second course — Benchmarking lessons

The most straightforward way to benchmark a novel computing paradigm [56] is by determining the resources (e.g., time) needed to meet a predefined target. There are different definitions of what this target should be (for example, a ground state or a particular energy value), however, there is consensus that the parameters of the device being benchmarked should be optimized. This is of importance, because sub-optimal parameter selection for smaller problems might lead to an apparent better scaling of the resources needed as a function of the problem size. As such, any claims for better performance and, in this case, *quantum speedup* could not be trusted. Alternatively, one could, for example, study the *quality* of the solutions found with a *fixed* amount of resources. Such an approach would, implicitly, remove the need to optimize parameters.

Probably one of the most problematic issues in assessing the near-term impact of quantum optimization machines is the definition of "*speedup*." Multiple teams have scrutinized theses devices [19, 52, 57, 20, 58, 21, 39, 59, 60, 22, 61, 62, 24, 41, 53, 26, 46, 63, 40, 31], however, to date, it remains controversial if there is any "*quantum speedup*" or not. Early on it was shown that random spin-glass benchmarks [58] on the sparse native D-Wave chimera topology might not be complex enough to observe any advantage [21, 24]. Therefore, efforts have shifted to synthetic spin-glass benchmark problems constructed using post-selection [24, 40, 64] methods, planted solutions [26, 31] or gadgets [30, 65]. Although some of the aforementioned results suggest that the commercially available D-Wave device has some advantage for carefully-designed synthetic problems, this advantage often was a constant speedup over other classical approaches, i.e., a similar scaling with the size of the input. Even worse, for a wide variety of these gadgets the logical structure of the underlying problem is easily decoded (e.g., via a decimation heuristic) and the remaining logical problem solved in polynomial time [28, 66] with exact methods. Therefore, any speedup claims are tentative, at best.

Definitions of quantum speedup – The first careful definition of quantum speedup was done in Ref. [23]. In particular, the authors of Ref. [23] differentiate between the following categories: *Provable quantum speedup*, *strong quantum speedup* (comparison to the best classical algorithm, regardless if the algorithm exists or not), *potential quantum speedup* (comparison to the best known classical algorithms), as well as *limited quantum speedup* (in this case, comparison against simulated quantum annealing via quantum Monte Carlo). In an effort to add more granularity to benchmarks, Ref. [28] introduced the notion of *limited sequential quantum speedup*, where comparisons are restricted to the best known *sequential* algorithms. Within this class, quantum annealers, as well as classically-simulated quantum annealers currently outperform all other known sequential algorithms for

different benchmark problems.

Slope vs offset – What would constitute a disruptive advantage of quantum annealers over classical optimization techniques? Purists might argue a change in the scaling (slope). This means that when analyzing the resource requirements (e.g., time to solve a problem) as a function of the number of variables, the growth of the requirements should be less pronounced than for classical hardware. However, what if the scaling is not better, but there is a constant offset that is several orders of magnitude? Likely, a constant offset of 10^4 would not be disruptive, because, using a parallel implementation of a classical algorithm on 10^4 compute cores is readily available, i.e., no disruptive advantage. However, what if this constant offset is 10^{12}? In that case, not only would we be out of luck with classical hardware, there would even be enough wiggle room to break up large problems that require more than 1000 qubits and solve them on the quantum hardware [67]. Still, to assess quantum speedup in the traditional sense, an improvement in the scaling is expected [68, 69].

Synthetic vs application speedup – The notion of speedup also strongly depends on the benchmark problem used. Although there have been indications of benchmark problems where the D-Wave 2000Q device [54] outperforms all known classical algorithms (without a visible scaling advantage), these are synthetic problems designed to "break" all known classical algorithms. A real-world application where quantum annealing outperforms all known classical algorithms remains to be found and would constitute a strong endorsement for quantum annealing to be a potentially disruptive technology.

Summarizing, it is argued that any claims for speedup should include *all* algorithms that are known to be amongst the best (see Refs. [6, 7, 8, 28, 66, 54] for an overview), as well as benchmarks from actual application problems. However, because application problems with a potential for a quantum advantage remain to be found, the development of synthetic spin-glass benchmarks will play a predominant role in the field. These should ideally have planted solutions, tunable typical computational complexity, impossible to deconstruct by tailored algorithms, and known to be hard for all currently known classical solvers [54]. The interplay between application-based and synthetic benchmarks, careful design of benchmarking strategies, clear definitions of speedup, as well as diligent use of statistics are key in assessing any potential future quantum speedup over classical technologies.

4. Entremet — Other benchmarking ideas

Because quantum annealers are designed to solve hard optimization problems fast, the benchmarking focus has been almost exclusively on speed. However, there are applications—for example molecular similarity in quantum chemistry [70], probabilistic membership filters [71], or machine learning—where a spectrum of uncorrelated solutions are more important than the actual optimum of the cost function. It was recently shown that vanilla quantum annealing with a transverse-field driver is a rather biased sampler [44]. If quantum annealing machines are expected to efficiently tackle these problems in the near future, efforts should shift to mitigate this currently existent exponential bias towards a subset of states. Therefore, in addition to assessing the speed of quantum annealing machines, an independent metric should be the fair sampling [44] capability of a particular device. Assuming near-uncorrelated solutions, a random unbiased sampler should find each solution of a degenerate problem with approximately the same probability (up to statistical fluctuations) [72]. Combined with sound quantum speedup benchmarks, this would represent a benchmarking gold standard for new hardware that uses different driving Hamiltonians, post-processing schemes, as well as applications that require different uncorrelated solutions.

5. Main course — Applications

As outlined in the introduction, multiple optimization problems across disciplines can be mapped onto spin-glass-like binary problems [32], up to a potential embedding overhead. If the community develops a notion of which types of problems have potential for a quantum advantage, tailored quantum optimization machines could be designed to tackle these. However, despite all efforts, a "killer" application or problem domain where quantum optimization excels has yet to be found.

What has been done? – NASA's Quantum Artificial Intelligence Lab has been a pioneer in the study of applications on current quantum annealing hardware. These applications range from spin glasses [46], to lattice protein models [73], fault diagnosis in graph-based systems [74] (e.g., circuits fault diagnosis [47]), operational planning [27], job-shop scheduling [75], and quantum-assisted machine learning [76], to name a few. In addition, different corporations such as 1QB Information Technologies (1QBit) have emerged, that aim at bringing novel computing techniques – such as quantum computing – to different enterprises. For example, 1QBit has studied different customer-driven application problems such as molecular similarity in chemistry [70] or the optimal trading trajectory problem [77]. These efforts have the largest potential in identifying problems that are well-suited for quantum annealing technologies, as well as for future digital programmable quantum computing systems.

Where vanilla quantum annealing likely won't work – Because transverse-field quantum annealing is a biased sampler [43, 44], it is unlikely that without fundamental changes to the hardware and driving

Hamiltonians quantum annealing will have an impact in applications that require an extensive sampling of a solution space with degenerate solutions. This means that current transverse-field implementations are unlikely to have any transformative impact in applications such as machine learning, inference, image recognition, probabilistic membership filters using SAT [71], or the optimization of the geometry of molecules in chemistry applications. However, future generations of these devices might include either better driver Hamiltonians or corrective post-processing schemes that might alleviate this problem. A recent example for post-processing of data was introduced in Ref. [78] and alleviates the biased sampling found in the D-Wave device.

Where the vanilla approach might work – Recently, D-Wave Systems Inc. demonstrated that their quantum annealing hardware can be used as a *physical simulator* [21, 79]. In that study, the machine's parameters were tuned to simulate a physical three-dimensional Edwards-Anderson Ising spin glass [80]. Current hardware with approximately 2000 qubits allows for the embedding of a three-dimensional quantum spin glass of 512 variables. The simulation of a quantum spin glass on traditional CMOS technology at low temperatures and with large transverse fields is notoriously difficult. By doubling the number of variables in the hardware the quantum annealer would be able to solve quantum spin-glass problems in a regime hard to probe for classical computers. Similarly, the machine could be used to study other phases of matter, such as frustrated pyrochlore magnets [81], simply by treating the Boolean variables as physical object. Although at first sight the application scope seems limited, not only are there multiple problems across condensed matter and statistical physics that should be revisited on an analog quantum simulator, but this would be the fulfillment of Richard Feynman's dream of a quantum simulator [82].

So how should the community proceed? First, a clear establishment of what properties of a problem and/or application make it well-suited for quantum optimization should be established. Tackle the quantum speedup problem from the bottom up by *first* understanding what makes a problem well-suited for quantum annealing and *then* building a special-purpose machine to solve it. In the medium to long term this will carve out the application scope of quantum annealing, as well as drive research and development in the right directions. Finally, although one could argue that simulated quantum annealing on CMOS technology might scale better than an analog quantum device, the offset between heuristics on CMOS and quantum hardware implementations remains huge. For example, in a recent study [30] the difference was approximately a factor of 10^7. Taking into account power consumption, this represents a sizable advantage for quantum annealing machines.

6. Cheese plate — Benefits for classical?

It is unlikely that classical CMOS technology will be fully replaced by quantum computing machines. For the next few decades, standard CMOS technology will still power most of humanity's computing needs from smartphones to servers while quantum computers will likely serve as large-scale co-processors in the cloud used for problems where classical would either require huge resources or quantum is optimally suited. In the near term, however, developments in quantum optimization have led to an "*arms race*" with classical technologies. Not only have there been many algorithmic advances, there has been a clear shift to custom silicon hardware.

Algorithmically, heuristics from the study of spin glasses have been adopted in the field of quantum optimization and, subsequently, by corporations interested in quantum and quantum-inspired optimization. State-of-the-art simulation approaches commonly used in the study of spin glasses are being adopted by industry. For example, replica exchange methods such as parallel tempering Monte Carlo [83, 84], particle swarm methods such as population annealing Monte Carlo [85, 86, 87], and cluster algorithms such as isoenergetic cluster moves [88] have been adopted by companies specialized in the optimization of binary problems [89]. In parallel, the emulation of quantum approaches on traditional hardware has led to the development of highly-efficient heuristics, such as simulated quantum annealing, that are becoming more commonplace both in academic, as well as industrial settings.

On the hardware side and driven by artificial intelligence applications, corporations are increasingly using field-programmable gate arrays (FPGAs) or custom hardware, such as Fujitsu's Digital Annealer [90] or Google Inc.'s Tensor Processing Unit, respectively. Furthermore, Microsoft has invested heavily in the development of highly-interconnected FPGAs via Project Catapult, a configurable cloud architecture. Such custom hardware cloud processing schemes set the stage for the eventual inclusion of quantum co-processors in the cloud. In the near-term, a hybrid classical-quantum cloud framework could be built with specific applications in mind. Eventually, once researchers are able to "predict" if a particular application is well suited for quantum approaches, more generic hybrid frameworks could be deployed. As emphasised in Sec. 5, gaining a deeper understanding of what makes a problem amenable for quantum (optimization) approaches should be in the center of current quantum computing research and hardware developments.

7. Dessert & Digestif — Concluding remarks

The development of synthetic benchmarking strategies based on Boolean frustrated systems will play a pivotal role

in the development of near-term quantum optimization machines. Furthermore, tools from the study of disordered and frustrated systems will play an increasing role in assessing the quantum-readiness of particular quantum computing applications. For the near term, quantum optimization using transverse-field quantum annealing on quadratic Hamiltonians will remain the standard. With all the insights gained by multiple researchers across fields, technology will be advanced further and—hopefully soon—to a point where quantum optimization has a clear application scope and outperforms classical computing technologies. If no true computational advantage can be found, either via a strong scaling advantage for a given application or a constant offset with a considerably smaller energy footprint than classical computing technologies, quantum annealing with a transverse field will likely fade away and be superseded by digital devices. Finding applications with even the weakest quantum speedup could give the quantum optimization field a massive boost that, in turn, will leverage other quantum computing developments, e.g., digital (where researchers will learn valuable lessons from analog developments). And these quantum computing developments will henceforth bolster the development of new classical computing technologies. It is this arms race that will herald a computing revolution.

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[69] A careful scaling analysis requires the precise optimization of all parameters in the optimization approach. Clearly, this poses a problem, because the optimization has to be run multiple times with different parameter settings to obtain the optimal set. Needless to say, this parameter optimization procedure should be included in the benchmarks, however, this is usually not the case. An alternative would be to use other time-independent metrics, such as residual energies or relaxed benchmarking approaches [24] that take the analog nature of quantum annealing machines into account.

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