Glassy Chimeras Could Be Blind to Quantum Speedup: Designing Better Benchmarks for Quantum Annealing Machines

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Recently, a programmable quantum annealing machine has been built that minimizes the cost function of hard optimization problems by, in principle, adiabatically quenching quantum fluctuations. Tests performed by different research teams have shown that, indeed, the machine seems to exploit quantum effects. However, experiments on a class of random-bond instances have not yet demonstrated an advantage over classical optimization algorithms on traditional computer hardware. Here, we present evidence as to why this might be the case. These engineered quantum annealing machines effectively operate coupled to a decohering thermal bath. Therefore, we study the finite-temperature critical behavior of the standard benchmark problem used to assess the computational capabilities of these complex machines. We simulate both random-bond Ising models and spin glasses with bimodal and Gaussian disorder on the D-Wave Chimera topology. Our results show that while the worst-case complexity of finding a ground state of an Ising spin glass on the Chimera graph is not polynomial, the finite-temperature phase space is likely rather simple because spin glasses on Chimera have only a zero-temperature transition. This means that benchmarking optimization methods using spin glasses on the Chimera graph might not be the best benchmark problems to test quantum speedup. We propose alternative benchmarks by embedding potentially harder problems on the Chimera topology. Finally, we also study the (reentrant) disorder-temperature phase diagram of the random-bond Ising model on the Chimera graph and show that a finite-temperature ferromagnetic phase is stable up to 19.85(15)% antiferromagnetic bonds. Beyond this threshold, the system only displays a zero-temperature spin-glass phase. Our results therefore show that a careful design of the hardware architecture and benchmark problems is key when building quantum annealing machines.

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I. INTRODUCTION

Quantum devices are gaining an increasing importance in everyday technology: They find applications in different technological areas such as (true) quantum random number generators, as well as quantum encryption systems for data transmission. The holy grail is to build a programmable quantum simulator with capabilities exceeding “traditional” computer hardware based on classical bits. The first programmable commercial device that attempts to exploit the unique power of quantum mechanics to perform computations is the D-Wave One quantum annealer [1]. In analogy to simulated annealing [2] where thermal fluctuations are adiabatically quenched to minimize a cost

function, this machine is based on the quantum annealing optimization method [3–11] where quantum fluctuations replace thermal ones.

Tests by different research teams suggest that, indeed, the D-Wave quantum annealer likely optimizes using quantum effects [12–16]. Although it has been shown theoretically [17], as well as with numerical experiments [8,18], that quantum annealing could, in principle, outperform classical (thermal) optimization algorithms (such as simulated annealing [2]) on an algorithmic level, when applied to a class of random edge-weight instances, the quantum annealing machine has not yet shown a speedup over classical optimization methods [13,19]. In this work, we present evidence for why this might be the case: The D-Wave One and Two quantum annealing machines use a restrictive “Chimera” topology (see Fig. 1 for an example with 128 quantum bits) imposed because of fabrication constraints of the solid-state quantum bits.

Probably the best benchmark problem to test the efficiency of optimization algorithms is a spin glass [20,21].

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FIG. 1. Example Chimera graph with $k^2 = 16$ blocks of 8 qubits (black dots). This means the system has $N = 128$ qubits and an effective linear size $L = \sqrt{N} = \sqrt{128}$. The high connectivity between the spins within each block effectively renders the model quasi-two dimensional. Note that the graph is not planar.

Both the disorder and frustration produce a complex energy landscape that challenges optimization algorithms. As such, all current benchmarks of the quantum annealing machine attempt to find the ground state of a certain class of Ising spin glass on the Chimera topology. However, as shown in this work, instances belonging to this class of Ising spin glasses on the Chimera topology only have a spin-glass phase at zero temperature. Furthermore, the energy landscape of such problems seems to be simpler down to low temperatures than for a system with a finite-temperature transition because correlations only build up very close to absolute zero. Because quantum annealing excels in tunneling through barriers—barriers that do not seem to be very pronounced at finite, but low temperatures in this case—classical annealing schedules might typically have an advantage for this particular class of systems.

Although the worst-case complexity of finding a ground state of an Ising spin glass on the Chimera topology is worse than polynomial [22], it seems that the fact that the system only orders at zero temperature allows for an easier determination of *typical* ground-state instances using heuristic classical approaches [13,23]. As such, Ising spin glasses on the Chimera topology live up to their name: an amalgamation of both ordinary and complex behavior.

We reach this conclusion by studying the critical behavior of Ising spin glasses with both Gaussian and bimodal random bonds on the Chimera topology, as well as the random-bond Ising model. Based on our findings, we propose stronger benchmark problems by embedding on the Chimera topology problems that should have a

finite-temperature transition and thus might be harder to optimize. Furthermore, our results show that a careful design of the hardware architecture and benchmark problems is key when building quantum annealing machines.

We should also mention that while the results of this paper provide a plausible explanation for the scaling behavior observed so far on random-bond Ising problems, it is also known that on quantum annealer implementations, the couplers and biases are influenced by various sources of noise and error, as demonstrated by the fact that gauge-transformed specifications of the same problem can give substantially different performance [13]. Classical simulated annealing does not, of course, have this issue, and it is currently unclear how much loss of efficiency these errors cause for the hardware.

The paper is structured as follows. In Sec. I we introduce the standard benchmark model. Results within the spin-glass sector are presented in Sec. II, followed by results within the ferromagnetic sector in Sec. III. In Sec. IV, we discuss better benchmarks, followed by concluding remarks.

II. MODEL, OBSERVABLES, AND ALGORITHM

We study the spin-glass Hamiltonian

$$\mathcal{H} = - \sum_{i,j=1}^N J_{ij} S_i S_j, \quad (1)$$

with $S_i \in \{\pm 1\}$ Ising spins on the nodes of the Chimera graph. An example of the topology with 4×4 blocks of 8 spins is shown in Fig. 1. A chimera graph with $k \times k$ blocks has $N = 8k^2$ spins and a characteristic linear length scale of $L = \sqrt{N}$. The interactions J_{ij} are either chosen from a Gaussian disorder distribution with zero mean and unit variance or from a bimodal distribution $\mathcal{P}(J_{ij}) = p\delta(J_{ij} - 1) + (1 - p)\delta(J_{ij} + 1)$, where with a probability p a bond is ferromagnetic.

Ordering in spin glasses is detected from the spin overlap $q = (1/N) \sum_i S_i^\alpha S_i^\beta$, where “ α ” and “ β ” are two independent spin replicas with the same disorder. In the ferromagnetic case, order is measured via the magnetization, i.e., $m = (1/N) \sum_i S_i^\alpha$. To detect the existence of a phase transition to high precision, we measure the Binder ratio [24] $g_O = (1/2)[3 - \langle \mathcal{O}^4 \rangle / \langle \mathcal{O}^2 \rangle^2]$, where $\mathcal{O}$ represents either the magnetization m for the ferromagnetic sector or the spin overlap q in the spin-glass sector. The Binder ratio is a dimensionless function, which means that, at a putative transition, data for different characteristic system sizes L will cross when $T = T_c$, where T_c is the critical temperature (up to corrections to scaling). This means $g_O \sim G_O[L^{1/\nu_O}(T - T_c^O)]$. Using a finite-size scaling analysis, the critical temperature T_c^O and the critical exponent ν_O can be determined. To uniquely determine the universality class of a system, two critical exponents are needed [25]. To this end, we also measure the susceptibility $\chi_O = N \langle \mathcal{O}^2 \rangle$,

where $\mathcal{O}$ again represents either the magnetization m for the ferromagnetic sector or the spin-glass order parameter q for the spin-glass sector. The susceptibility scales as $\chi_{\mathcal{O}} \sim L^{2-\eta_{\mathcal{O}}} C_{\mathcal{O}} [L^{1/\nu_{\mathcal{O}}}(T - T_c^{\mathcal{O}})]$, where $\eta_{\mathcal{O}}$ is an independent critical exponent.

Simulations are done using the replica exchange Monte Carlo [26] method, and simulation parameters are listed in Table I. Note that for each disorder instance, we

TABLE I. Simulation parameters: For each number of spins N and fraction of ferromagnetic bonds p , we equilibrate and measure for 2^b Monte Carlo sweeps. $T_{\min}$ [$T_{\max}$] is the lowest [highest] temperature, and N_T is the number of temperatures. N_{sa} is the number of disorder samples. The bottom block labeled with “Gauss” lists the simulation parameters for the pure spin glass with Gaussian disorder. The numbers for the pure spin glass with bimodal disorder are labeled with “ $p = 0.500$.”

p	N	b	$T_{\min}$	$T_{\max}$	N_T	N_{sa}
0.000	800	21	2.500	5.500	31	128
0.000	1152	21	2.500	5.500	31	128
0.000	1568	21	2.500	5.500	31	128
0.000	2048	21	2.500	5.500	31	128
0.000	2592	21	2.500	5.500	31	128
0.000	3200	21	2.500	5.500	31	128
0.040, 0.080, 0.120	800	21	2.500	5.500	31	2800
0.040, 0.080, 0.120	1152	21	2.500	5.500	31	2800
0.040, 0.080, 0.120	1568	21	2.500	5.500	31	2800
0.040, 0.080, 0.120	2048	21	2.500	5.500	31	2800
0.040, 0.080, 0.120	2592	21	2.500	5.500	31	2800
0.040, 0.080, 0.120	3200	21	2.500	5.500	31	2800
0.160, 0.180, 0.190	800	21	1.500	4.500	31	2800
0.160, 0.180, 0.190	1152	21	1.500	4.500	31	2800
0.160, 0.180, 0.190	1568	21	1.500	4.500	31	2800
0.160, 0.180, 0.190	2048	21	1.500	4.500	31	2800
0.160, 0.180, 0.190	2592	21	1.500	4.500	31	2800
0.160, 0.180, 0.190	3200	21	1.500	4.500	31	2800
0.195, 0.197	800	21	0.500	3.500	31	2800
0.195, 0.197	1152	21	0.500	3.500	31	2800
0.195, 0.197	1568	21	0.500	3.500	31	2800
0.195, 0.197	2048	21	0.500	3.500	31	2800
0.195, 0.197	2592	21	0.500	3.500	31	2800
0.195, 0.197	3200	21	0.500	3.500	31	2800
0.200, 0.220	800	21	1.500	4.500	31	2800
0.200, 0.220	1152	21	1.500	4.500	31	2800
0.200, 0.220	1568	21	1.500	4.500	31	2800
0.200, 0.220	2048	21	1.500	4.500	31	2800
0.200, 0.220	2592	21	1.500	4.500	31	2800
0.200, 0.220	3200	21	1.500	4.500	31	2800
0.500	512	21	0.212	1.632	30	5964
0.500	648	24	0.212	1.632	30	5323
0.500	800	24	0.212	1.632	30	4859
0.500	1152	21	0.373	1.377	21	1140
Gauss	512	21	0.212	1.632	30	5000
Gauss	648	24	0.212	1.632	30	5149
Gauss	800	24	0.212	1.632	30	5053
Gauss	1152	24	0.212	1.632	30	1326

simulate two independent replicas to compute the spin-glass overlap. In the Gaussian case, we test equilibration using the method developed in Ref. [27] adapted to the Chimera topology. For bimodal disorder, we perform a logarithmic binning of the data. Once the last four bins agree within error bars, we deem the system to be in thermal equilibrium. To obtain optimal values for the critical parameters, we determine these via the analysis method pioneered in Ref. [28], where the critical parameters are optimized using a Levenberg-Marquard minimization until the chi square of a fit to a third-order polynomial is minimal. This approach is then bootstrapped to obtain statistically sound error bars.

III. RESULTS WITHIN THE SPIN-GLASS SECTOR

Figure 2 shows a finite-size scaling analysis of the Binder ratio (top panel) for both Gaussian disorder (full

FIG. 2. Top panel: Finite-size scaling of the Binder parameter g_q as a function of $T(\sqrt{N})^{1/\nu_q}$ for both Gaussian (full symbols) and bimodal (open symbols) disorder on the Chimera topology. The data scale very well for $T_c^q = 0$ and $\nu_q = 4$ in both cases. Bottom panel: Finite-size scaling of the spin-glass susceptibility χ_q for both Gaussian and bimodal disorder. Plotted are $\chi_q/(\sqrt{N})^{2-\eta_q}$ vs $T(\sqrt{N})^{1/\nu_q}$. The data scale very well for $T_c^q = 0$, $\nu_q = 4$, and $\eta_q = 0$. Note that there is no universality violation. Error bars are smaller than the symbols.

symbols) and bimodal disorder with $p = 0.50$ (open symbols) in a semilogarithmic scale. The data scale extremely well, even far from the spin-glass transition temperature. We find that for both cases, we have the same critical parameters, namely [29],

$$T_c^q = 0, \quad \nu_q \approx 4, \quad \eta_q \approx 0. \quad (2)$$

Note that spin glasses on two-dimensional square lattices have $\nu \approx 3.45$ [30]; i.e., spin glasses on the Chimera topology are close to two space dimensions.

Interestingly, the phase transition to a spin-glass phase only occurs at zero temperature, despite the Chimera graph being nonplanar. Furthermore, the divergence of the correlation length is rather violent, with $\xi \sim T^{-4}$ for $T \rightarrow 0$. This suggests that the phase space and correlations only build up close to $T = 0$ for a spin glass defined on the Chimera topology. One of the potential advantages of a quantum algorithm over a classical one lies in its ability to tunnel through barriers. Classical algorithms must “climb” over these barriers [31]. The aforementioned results imply that the barriers of a spin glass defined on a Chimera graph at nonzero temperature seem to be of “finite” height, while for any Ising spin glass with a finite transition temperature, the barriers diverge below T_c^q for decreasing temperature T and increasing system size N . This could offer one explanation for why quantum annealing machines, such as D-Wave One and Two, cannot find a noticeable speedup over classical algorithms such as vanilla simulated annealing [2] on this class of problems. Furthermore, a spin glass on a Chimera graph seems to order in an almost “discontinuous” fashion at zero temperature with the highly connected blocks of eight spins behaving like a “super spin” on a two-dimensional-like planar lattice. Once the individual blocks order, the whole system suddenly orders. It is well known that quantum annealing has problems when first-order transitions are present [32–35]; i.e., this could be the second reason why quantum annealing machines do not seem to outperform simple classical optimization methods on these problems.

IV. RESULTS WITHIN THE FERROMAGNETIC SECTOR

For completeness, we also study the Ising ferromagnet on the Chimera graph and compute the disorder p (fraction of ferromagnetic bonds) vs temperature T phase diagram of the model. For no disorder, i.e., the pure ferromagnet where $J_{ij} = 1 \quad \forall i, j$ in Eq. (1), an Ising model on the Chimera graph displays a two-dimensional-Ising-model-like behavior. Figure 3, top panel, shows a finite-size scaling analysis of the ferromagnetic Binder ratio g_m as a function of the scaling variable $(\sqrt{N})^{1/\nu_m}(T - T_c^m)$. The data scale extremely well for $T_c^m = 4.1618(3)$ and $\nu_m = 1$. Note that the obtained value for the critical exponent ν_m agrees with the value for the two-dimensional Ising ferromagnet [25],

therefore corroborating our assumption that the system might behave similarly to a two-dimensional superspin Ising model.

Figure 3, bottom panel, shows a finite-size scaling analysis of the ferromagnetic susceptibility $\chi_m/(\sqrt{N})^{2-\eta_m}$ as a function of $(\sqrt{N})^{1/\nu_m}(T - T_c^m)$ using the estimate of the critical temperature determined from the finite-size scaling of the Binder ratio. The data scale very well with very small corrections to scaling using $\nu_m = 1$ and $\eta_m = 2/5$. Note that the value of the critical exponent η_m is slightly larger, yet close to the exact value of the two-dimensional Ising model ($\eta = 1/4$). Therefore, an Ising ferromagnet on the Chimera graph and the two-dimensional Ising model do not share the same universality class [36]. In summary,

$$T_c^m = 4.1618(3), \quad \nu_m \approx 1, \quad \eta_m \approx 2/5. \quad (3)$$

FIG. 3. Top panel: Finite-size scaling of the ferromagnetic Binder parameter g_m as a function of $(\sqrt{N})^{1/\nu_m}(T - T_c^m)$ and $p = 0$ (pure ferromagnet) on the Chimera topology. The data scale very well for $T_c^m = 4.1618(3)$ and $\nu_m = 1$. Bottom panel: Finite-size scaling of the ferromagnetic susceptibility χ_m . Plotted are $\chi_m/(\sqrt{N})^{2-\eta_m}$ vs $(\sqrt{N})^{1/\nu_m}(T - T_c^m)$. The data scale very well for $T_c^m \approx 4.1618(3)$, $\nu_m = 1$, and $\eta_m = 2/5$. Error bars are smaller than the symbols.

FIG. 4. The disorder p vs temperature $T = T_c^m$ phase diagram for the random-bond Ising model defined on the Chimera graph. The (blue) dotted line represents the Nishimori line. The red (solid) line is a guide to the eye. Under the solid curve, the system orders ferromagnetically (FM). For $p \geq p_c \approx 0.1985(15)$, ferromagnetic order is lost and the system is paramagnetic (PM). For $p \gtrsim p_c$ and $T = 0$, there is a zero-temperature spin-glass state [37].

Finally, we study the random-bond version of the Ising model on the Chimera graph where a fraction p of ferromagnetic bonds is antiferromagnetic. We vary p and compute the critical temperature of the ferromagnetic phase. Figure 4 shows the (critical) temperature T vs disorder p phase diagram. The dotted (blue) line represents the Nishimori condition [40] $\exp(-2\beta) = p/(1-p)$. At the point where the phase boundary (solid line) crosses the Nishimori line, i.e., for $p > p_c = 0.1985(15)$, ferromagnetic order is lost. This means that for any finite temperature and $p \leq p_c$, a random-bond Ising model on the Chimera graph is essentially a disordered ferromagnet and is easily solved with a conventional optimization algorithm. Therefore, to compare a quantum adiabatic optimizer to any classical optimization method, strong enough disorder is needed.

V. DISCUSSION

Figure 5 shows cartoons of the energy landscape for a system with a zero-temperature transition [panel (a), top] and a finite-temperature transition [panel (b), bottom] to a spin-glass state. When the temperature is above the putative critical temperature T_c , the energy landscape is typically simple with one dominant minimum. For a system that has a finite-temperature transition and for temperatures $T < T_c$, the energy landscape becomes rough with barriers that grow with decreasing temperature T and increasing system size N until the ground state of the system is reached. However, for a system where $T_c = 0$, such as spin glasses on the Chimera topology, the energy landscape is likely much simpler until close to the ground state. This means that for such a system, a classical annealing schedule

FIG. 5. Sketch of the (coarse-grained) energy landscape for a system with a zero-temperature transition [panel (a), top] and a finite-temperature transition [panel (b), bottom] to a spin-glass state. For high enough temperatures, i.e., above the critical temperature T_c , the energy landscape is simple, with one clear minimum that dominates and some “bumps along the way.” For a system that has a finite-temperature transition and for temperatures $T < T_c$, the energy landscape becomes rough, with clear barriers that render any classical annealing schedule inefficient because the system can easily be trapped in a metastable state for decreasing temperature. These barriers grow with increasing system size N and decreasing temperature T until they form a rough energy landscape for $T = 0$ (ground state of the system). For a system where $T_c = 0$, such as spin glasses on the Chimera topology, the energy landscape is typically simpler up until the ground state is reached. This means that for such a system, a classical annealing schedule like simulated annealing should perform better in comparison to quantum annealing, which excels when the energy landscape exhibits barriers [41].

should perform well in comparison to quantum annealing, which, in theory, excels when the energy landscape has diverging barriers. Note also that when the system with bimodal disorder is in the ferromagnetic phase ($p < p_c$), the energy landscape is also simpler and reminiscent of the cartoon shown in the left-most panels of Fig. 5. This means that benchmarking quantum annealing machines that operate at low, but finite temperatures using spin glasses on a Chimera topology is likely not the best approach. Indeed, recent studies in a field [51,52] have shown that spin-glass instances can be efficiently computed classically, albeit still scaling exponentially. However, because there is likely no spin-glass state in a field [53–56], this is no surprise. To truly discern if quantum annealing machines (defined on the Chimera topology) display an advantage over classical annealing algorithms, problems that display a finite-temperature transition and have a rough energy landscape for a range of finite temperatures need to be embedded in the machine’s topology. Given the current hardware constraints, we propose the following benchmarks.

Three-dimensional cubic lattices.—The system has a finite-temperature transition to a spin-glass state at $T_c \approx 0.96J$ for Gaussian disorder ($T_c \approx 1.1J$ for bimodal disorder and $p = 0.5$) [28]. We estimate that a Chimera graph of 2048 qubits could be used to embed a relatively

modest 3D system of $5^3 = 125$ spins with periodic boundary conditions and one of size $8^3 = 512$ with free boundary conditions. Note that current state-of-the-art classical optimization algorithms [57,58] can estimate ground states to high accuracy of up to approximately $14^3 = 2744$ spins.

Viana-Bray model.—The Ising spin glass is defined on a random graph with average connectivity k [27,59]. For any $k > 2$, the system has a finite-temperature phase transition into a spin-glass state. To simplify the embedding, a random graph with Gaussian disorder and $k = 3$ could be studied, where $T_c \approx 0.748J$. However, to be able to embed the long-range connections between the spins, we estimate that $\mathcal{O}(N^2)$ qubits might be needed to embed a system with N spins like in the mean-field Sherrington-Kirkpatrick model [60–62].

Rescaled Chimera systems.—It is plausible that if the ratio of interactions within the cells and between the cells changes proportional to the system size, a mean-field-like finite-temperature spin-glass transition might emerge. For example, the random intercell interactions could be rescaled with $J_{ij} \rightarrow J_{ij}/f(N)$ [where $f(N)$ is a nondecreasing function of the system size] while leaving the random intracell interactions untouched. We attempted to weaken the effects of the tightly bound intercell spin clusters in the Chimera graph by setting the spin-spin interactions to $1/4$ of all intracell interactions (on average). Although universality considerations would suggest that T_c should still be zero when $f(N) = 1/4 \quad \forall N$, our data for systems up to approximately 3200 spins suggest $T_c \approx 0.6(2)$. We do emphasize, however, that corrections to scaling are huge and a study with far larger systems might be needed.

One could, in principle, also embed a two-dimensional Ising spin glass on a square lattice, where it was first shown by Santoro *et al.* that quantum annealing might display an advantage over classical annealing via simulations at very low temperatures [8]. However, ground states of two-dimensional Ising spin glasses can be computed in polynomial time, and the low-temperature behavior of this system is known to be unusual and still controversial [63]. As such, this might not be a robust and well-controlled benchmark, especially because the D-Wave machines operate at temperatures considerably higher than in the aforementioned study by Santoro *et al.* [8].

The previous examples also illustrate a limitation of the Chimera topology: To embed many systems, a large overhead of quantum bits in the machine to simulated physical bits is needed. This is particularly the case because no long-range connections between the spins are present—a feature that should be included in future chip designs. Finally, at this point it is unclear if the critical behavior of an *embedded* system is the same as the critical behavior of the *actual* classical system. This is of utmost importance if one wants to use programmable quantum annealing machines as quantum simulators.

VI. CONCLUSIONS

Although Barahona [22] has rigorously shown that spin glasses defined on graphs like the Chimera topology are worst-case NP-hard types, the Chimera spin glass of the type used so far to compare quantum to classical annealers represents a hard, but typically easier optimization problem. Because such a spin glass on the Chimera topology only orders at zero temperature, classical thermal annealers will typically be able to efficiently estimate ground states for the system. The performance of these classical algorithms would considerably deteriorate if the problem to be optimized exhibits a finite-temperature transition below which energy barriers diverge with decreasing temperature and increasing system size. To be able to show that quantum annealing machines based on the Chimera topology outperform classical annealing schedules, nontrivial embeddings in higher space dimensions or with long-range interactions, as outlined above, are needed. Furthermore, at this point it is unclear how the overhead of the embedding scales with the size of the system and if the embedded system via edge contraction shares the same universality class as the true problem to be emulated—especially when simulated on the actual D-Wave hardware [64]. The latter open questions are the subject of current research, and we conclude by emphasizing that the design of the hardware topology in quantum annealing machines is of crucial importance.

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