The power of pausing: advancing understanding of thermalization in experimental quantum annealers

Jeffrey Marshall,1,2,3 Davide Venturelli,1,4 Itay Hen,3,5 and Eleanor G. Rieffel4

1 USRA Research Institute for Advanced Computer Science, Mountain View, California 94035, USA
2 USRA NAMS Quantum Academy R&D Student Program, NASA Ames Research Center, Mountain View, California 94035, USA
3 Department of Physics and Astronomy, and Center for Quantum Information Science & Technology, University of Southern California, Los Angeles, California 90089, USA
4 QuAIL, NASA Ames Research Center, Moffett Field, California 94035, USA

We investigate alternative annealing schedules on the current generation of quantum annealing hardware (the D-Wave 2000Q), which includes the use of forward and reverse annealing with an intermediate pause. This work provides new insights into the inner workings of these devices (and quantum devices in general), particular into how thermal effects govern the system dynamics. We show that a pause mid-way through the anneal can cause a dramatic change in the output distribution, and we provide evidence suggesting thermalization is indeed occurring during such a pause. We demonstrate that upon pausing the system in a narrow region shortly after the minimum gap, the probability of successfully finding the ground state of the problem Hamiltonian can be increased by several orders of magnitude. We relate this effect to relaxation (i.e., thermalization) after diabatic and thermal excitations that occur in the region near to the minimum gap. For a set of large-scale problems of up to 500 qubits, we demonstrate that the distribution returned from the annealer very closely matches a (classical) Boltzmann distribution of the problem Hamiltonian, albeit one with a temperature at least 1.5 times higher than the (effective) temperature of the annealer. Moreover, we show that larger problems are more likely to thermalize to a classical Boltzmann distribution.

I. INTRODUCTION

Inspired by thermal annealing and by the adiabatic theorem of quantum mechanics, quantum annealers are designed to make use of diminishing quantum fluctuations in order to efficiently explore the solution space of particular discrete optimization problems. In the last few years, chip sizes have grown in accordance with Moore’s law, and current devices contain on the order of 2000 superconducting qubits, potentially allowing for relatively large scale problems to be solved. Though progress has been made [1, 2], whether quantum annealing provides a speedup [3, 4] over conventional approaches to optimization remains open. Alternatively, researchers have suggested that quantum annealers may be useful for thermal sampling tasks [5–8], such as the NP-hard problem of sampling from a Boltzmann distribution, which has application in machine learning and artificial intelligence. Early results and theory exist [6, 7, 9], but the extent to which thermalization occurs in quantum annealing remains a hotly contested issue.

We take advantage of two advances to further understand the behavior of quantum annealers and the distributions they output. The first is the introduction of new features that support a wider variety of annealing schedules on the D-Wave 2000Q quantum annealers; the only schedule parameter earlier machines provided was setting the total anneal time, and thereby the speed with which the default annealing schedule was traversed. Specifically, we make use of the new pause feature, which allows one to pause the anneal, keeping the strengths of the driver Hamiltonian and the problem Hamiltonian constant for extended periods of time (up to ∼1ms), before completing the default annealing schedule. We also make use of the reverse annealing feature, which allows one to start in a classical state with the strength of the problem Hamiltonian and the driver Hamiltonians what they would be at the end of the default anneal, and to then increase the strength of the driver Hamiltonian and reduce that of the problem Hamiltonian, following the default schedule in reverse, up until a point at which one then anneals forward according to the default schedule, possibly pausing between the reverse and forward anneals. The second advance we rely on is new entropic sampling techniques based on population annealing that enable accurate estimates (i.e., with quantifiable error) of the eigenspectrum degeneracies for large-scale (e.g., 500 qubits) planted-solution problems [8, 10].

We surveyed the performance of the quantum annealer on two problem classes, studying the output of the device under an anneal with an intermediate pause inserted at different locations during the anneal, and for differing pause lengths. The first problem class contains 12-qubit problems for which we can compute exactly the eigenspectrum throughout the anneal. The second class contains planted-solution problems, for which entropic sampling provides accurate estimates of the spectrum degeneracies for the problem Hamiltonian, with hundreds of qubits (see Appendix C for more information). We found that a pause can increase the performance by orders of magnitude when the pause occurs within a well defined, relatively narrow region of the anneal, but has little effect if placed outside that region. This effect, and the location of the best region for pausing, is remarkably ro-
bulk across instances within a class, pause lengths, and total annealing times. We interpret the results with a phenomenological model that takes into account the relevant time scales involved in the annealing process, and also used the reverse anneal feature to further investigate these phenomena. This picture suggests that a pause is effective after the minimum gap, and after thermal excitations start to diminish, but while the driver is still strong enough and the eigenvalues of the Hamiltonian are not too far apart so that significant dynamics can still take place. This picture differs greatly from that for closed system adiabatic quantum computing for which a pause would be most effective at the minimum gap. For the 12-qubit problems, we were able to compute the location of the minimum gap and confirm our open system picture.

We then turned to the question of how Boltzmann the final distributions are. For the 12-qubit problems, we compared the final distribution with the projected (onto the computational basis) quantum Boltzmann distributions for the full Hamiltonian at all points along the anneal. The final distribution fit reasonably well to the projected quantum Boltzmann distribution at the optimal pause location and at the device’s operating temperature. Outside this parameter range the fit was poor. For planted-solution problems, equipped with the energy spectrum degeneracies of the problem, we compared the final distribution with the classical Boltzmann distribution of the problem Hamiltonian. Here, we found a strong correlation ($R^2 > 0.9$) for all instances and pause locations, with the correlations becoming even stronger as the problem size increased and as a pause was added, with the best fit being at the optimal pause location, but for a higher temperature than might be expected.

We conclude with a discussion of these results, and a call for a deeper theory that can make quantitative predictions about the optimal pause location, the location of the best fit projected Boltzmann distribution, the best fit location and temperature for fit with a classical Boltzmann distribution for the problem Hamiltonian, as well as experimental investigation of these phenomena for other problem classes. The observations we make are relevant not only for quantum annealers, but for any quantum device which is non-negligibly coupled to a thermal environment, thus shedding light on fundamental physical processes involved across a broad range of devices. We begin by reviewing some background material before presenting our results and discussing their interpretation and implications.

### A. Background

Transverse field quantum annealing evolves the system over rescaled time $s = t/t_a \in [0,1]$, where $t$ is the time, and $t_a \in [1,2000] \mu s$ the total run-time (chosen by the user). We will occasionally refer to the rate of the anneal $ds/dt$ which on the D-Wave 2000Q can be set to zero during the pause or take values in interval $ds/dt \in [0.0005,1] \mu s^{-1}$ otherwise. The time-dependent Hamiltonian is of the form

$$H(s) = A(s)H_d + B(s)H_p,$$

where $H_p = \sum_{\langle i,j \rangle} J_{ij} \sigma_i^z \sigma_j^z + \sum_i h_i \sigma_i^z$ is the programmable Ising spin-glass problem (the final Hamiltonian) to be sampled defined by the parameters $(J_{ij}, h_i)$, and $H_d = -\sum_i \sigma_i^z$ is a transverse-field (or ‘driver’) Hamiltonian which provides the quantum fluctuations (the initial Hamiltonian). Here $N$ is the total number of qubits in the problem, and $\langle i, j \rangle$ indicates the sum is only over a coupled qubits, defined by the hardware ‘chimera’ graph (see Fig. 24 of Appendix D). The device we use, the D-Wave 2000Q contains $16 \times 16$ unit cells each containing 8 qubits, thus having a maximum of 2048 qubits. However, because of some faulty qubits/couplers, the actual number of operating qubits is 2031. These ‘dead’ qubits appear randomly dispersed throughout the hardware graph.

The initial state is fixed as the ground state of $H_d$, $|\psi(0)\rangle = |+\rangle^\otimes N$ where $|+\rangle = \frac{1}{\sqrt{2}} (|0\rangle + |1\rangle)$ (defined in the computational basis via $\sigma = |1\rangle \langle 1| - |0\rangle \langle 0|)$). The manner in which the Hamiltonian is evolved in time is determined by the annealing schedule (i.e. the time dependence of $A, B$). The default schedule for the D-Wave 2000Q is shown in Fig. 1.

After an annealing run, the system is measured in the computational basis. Performing many such runs allows statistics about the annealer to be collected; useful measures include the probability of successfully finding the ground-state of $H_p$ (which is the solution to a classical optimization problem) which we denote as $P_0$, or the average energy returned ($E$).

One way to provide more robust statistics, is by changing the ‘gauge’ of the problem. This is a trivial re-mapping of the problem so as to avoid certain biases which may be present for certain couplers/qubits (e.g., some couplers may have fewer analog control errors associated with programming in $J = +1$ as compared to $J = -1$, or certain qubits may be more likely to align with $+z$ as compared to $-z$ even in the absence of any fields). The mapping involves changing the couplings/fields as $J_{ij} \rightarrow J_{ij} r_i r_j, h_i \rightarrow h_i r_i$, where $r = (r_1, \ldots, r_N)$ is a vector of random entries $r_i \in (-1,1)$. Notice any configuration $\vec{s} = (s_1, \ldots, s_N)$ has a corresponding configuration of the mapped problem $\vec{r} = (r_1 s_1, \ldots, r_N s_N)$ with the same cost, thus the problem itself is exactly the same.

An important quantity identified in Ref. [11] is the ratio between the strength of the driving Hamiltonian and the problem Hamiltonian, $Q(s) := A(s)/B(s)$, shown in Fig. 2 for the D-Wave 2000Q schedule. Also important are the classical thermal fluctuations which are governed by the quantity $C(s) := k_B T / B(s)$, where $T$ is the temperature of the annealer. Observing the relative scales
FIG. 1. Annealing schedule in GHz (units of $h = 1$). The operating temperature ($T = 12.1$ mK, or equivalently 0.25 GHz) of the chip is also shown (black-dashed line).

FIG. 2. Dimensionless annealing schedule. We plot the ratio $Q(s) := A(s)/B(s)$, and the ratio of the operating temperature ($T = 12.1$ mK) to the strength of the problem Hamiltonian, $C(s) := k_B T / B(s)$.

of the characteristic energies associated to the driving terms (i.e. transverse field, environmental bath) with the energy of the problem Hamiltonian allows us to infer the existence of different regimes where a given process becomes energetically dominant. In particular, i) at early times when $Q \gg C > 1$, and the system mostly remains in the ground state of $H$, ii) when $Q \sim C \sim O(1)$ and non-trivial dynamics occur with $H_d$ driving various transitions between computational basis states, and iii) $Q \ll C \ll 1$ when the Hamiltonian is mostly diagonal (in the computational basis) and little population transfer occurs between the eigenstates (the ‘frozen’ region) through diabatic transitions. Thermal transitions could occur but those depend also on the strength of the coupling to the thermal bath (see below).

B. Adapting the standard annealing schedule

The current generation of hardware, the D-Wave 2000Q, allows users to tweak the default schedule in various ways. In particular this gives one the ability to:

1) Pause the evolution at some intermediate point $s_p < 1$ in the anneal, for time $t_p$.

2) Perform reverse annealing, where the system is initialized in a classical configuration at time $s = 1$, evolved backwards to an earlier time $s_p < 1$ before evolving the system back to time $s = 1$ where a read-out occurs. Additionally, a pause can be inserted between the two evolutions.

3) Speed-up or slow-down the schedule during intermediate intervals of the anneal.

4) Provide per-qubit annealing offsets.

Fig. 3 shows an example of an annealing schedule with a pause, and also an example of a reverse annealing schedule.

Based on these features, new methods of sampling from an annealer have been developed and proposed, such as exploiting reverse annealing to explore the energy landscape in a novel manner [12–16]. Moreover, performance advantages have been observed by offsetting the fields of some of the qubits, allowing one to evade spurious transitions which occur during the minimum gap [17, 18].

This paper focuses on the first capability listed above, where we embed a pause in the default annealing schedule, i.e., the Hamiltonian is fixed at $H(s_p)$ for lengths of time chosen by the user. This approach enables us to study key mechanisms determining the output of the annealer, such as thermalization, and to identify key regimes of the anneal (as discussed in Sect. II B). To further confirm our explanation for the behavior of the system, we use reverse annealing in a similar way, inserting pauses of varying lengths at differing locations.

C. Theory

Naively, one might expect the final distribution at the end of the anneal to be a classical Boltzmann distribution for the problem Hamiltonian $H_p$ at the operating temperature of the device, specifically, $\rho \sim \exp(-\beta B(1) H_p)$, where $\beta = 1/k_B T$, with $T$ the operating temperature of the annealer (on the order of 10-20mK in the various generations of D-Wave annealers). But it has long been known that this is not the case. The freeze-out hypothesis due to Amin [5] suggests that while early in the anneal the system thermalizes, later in the anneal, at an instance dependent, but temperature independent,
The transverse field drives transitions between eigenstates of the transverse field Hamiltonian. The figure shows an example of annealing parameter $s$ as a function of time $t$ for an anneal with a pause, for both forward and reverse annealing. Here a 1 µs pause ($t_p = 1$ µs) is inserted into the annealing schedule at $s_p = 0.5$ (i.e., at $t = 0.5$ µs), which otherwise has a total anneal time of $t_a = 1$ µs.

Freezing-out point, the transverse field strength has diminished and the gap between eigenvalues increased to the point that the transition matrix elements are so small that essentially no dynamics happen after this “freeze-out” point. This hypothesis predicts that, for instances with well-defined freeze-out points, the final distribution would indeed be a classical Boltzmann distribution for $H_p$ but at a higher “effective temperature” corresponding to the freeze-out point. More specifically, the theory hypothesizes a freeze-out point $s^*$ that occurs once $Q(s^*)$ and $C(s^*)$ are so ‘small’ that the time-scale upon which the transverse field drives transitions between eigenstates of $H_p$ is much longer than the system evolution time, hence little population transfer occurs. The expected distribution would then be close to $\rho \sim \exp(-\beta B(s^*) H_p)$ [5, 11]. The paper proposing this hypothesis [5] recognized that a well-defined freeze-out point will only exist under certain circumstances, with more recent debate as to how typically those circumstances hold.

Taking inspiration from work that addressed an open-system treatment in the weak coupling regime for general problems [19], and in the non-perturbative regime for specific problems [20, 21], we look at transitions between instantaneous energy levels $E_i(s) > E_j(s)$ that are governed by Fermi’s Golden Rule rate $\Gamma_{ij}$ (ignoring for convenience the spectral density term):

$$\Gamma_{ij}(s) \propto \sum_{k, \alpha} g_{\alpha}^2 |\langle E_i(s) | \sigma_{\alpha k}^\alpha | E_j(s) \rangle|^2 \frac{1}{1 - \exp(-\beta |E_i(s) - E_j(s)|)},$$

(2)

where $g_{\alpha}$ is the environment coupling strength to the $\alpha = x, y, z$ component of the system spins, and $\sigma_{\alpha k}^\alpha$ is the $\alpha$ Pauli operator acting on the $k$-th spin. The explanation of freeze-out in this picture is that as $s \to 1$, energy gaps $|E_i - E_j|$ open up, as well as the matrix elements $\langle E_i(s) | \sigma^\alpha | E_j(s) \rangle \to 0$ (which is typically the dominant environment-spin coupling [21–23]) as the Hamiltonian becomes more diagonal in the $z$-basis, thus the transition rates dramatically slow down late in the anneal. Therefore, the two strongest (possibly competing) effects determining the relaxation rate Eq. (2) are the instantaneous energy gap, and $Q(s)$ (via the matrix element).

Marshall et al. [11] used annealers operating at two different temperatures to corroborate the freeze-out hypothesis, finding consistency in the freeze-out point location for instances with well defined freeze-out points late in the anneal. On the negative side, however, this study showed that the most instances did not fall into this category, leaving open whether one would even expect the final distribution to be a classical Boltzmann distribution for $H_p$, in the typical case.

With the new entropic sampling techniques, and the new pause and reverse annealing capabilities on the D-Wave 2000Q quantum annealer, it is now possible to develop a better understanding of the final distributions returned and the extent to which thermalization happens along the way. Before describing the results, we discuss a qualitative theory in terms of key time scales involved in open-system quantum annealing. The key time scales we consider are:

- the pause time scale $t_p$, the length of the pause inserted into the annealing schedule,
- the relaxation time scale $t_r$, related to the inverse of Eq. (2), and
- the Hamiltonian evolution time scale, $t_H(s) \sim t_a \left| \frac{dH(s)}{ds} \right|^{-1}$, which is the characteristic time upon which the system Hamiltonian $H(t)$ changes. This quantity depends on both $t_a$ and the parameters $A(s)$ and $B(s)$.

Fig. 4 provides a schematic illustration of four regions within an anneal which one would expect have qualitatively different dynamics. In the figure, we plot $t_H$ as a straight line only for convenience. Early in the anneal, the eigenvalues are spread, with $E_i - E_0 \gg 0$, and with the system starting the ground state state, one expects little in the way of dynamics and the probability that the system is in the instantaneous ground state to be high, $P_0 \approx 1$. Once the eigengaps decrease sufficiently to be within the Hamiltonian evolution time scale, we expect to see thermal excitations, with sufficient dynamics that the system instantaneously thermalizes. As we leave this region, the energy gaps open, and the strength of the driver Hamiltonian reduces so that instantaneous thermalization no longer takes place, but transitions still occur. This region is relatively narrow since $t_r$ increases exponentially as the gaps open up. It is in this region that we expect a pause to aid thermalization and thereby substantially improve solution probability. Near the end of the anneal, with the gap distances becoming very large,
and where very little transverse field is applied, one would expect that the dynamics are effectively frozen.

II. RESULTS

Throughout this work we consider problems of two different types:

1. To study large problems, we work with problems of the planted-solution type [25], such as the $I_{783}$ instance of Fig. 5. We chose these problems, because recent techniques enable us to know in advance the general analytic form of the spectrum of $H_p$, including the ground state, as well as certain information about the degeneracy of the energy levels (see Appendix C).

2. To analyze problems with respect to spectral properties of the full Hamiltonian, $H(s)$, we used 12-qubit problems, where $J_{ij} \in [-1, 1]$ (uniformly random).

In both cases, we used zero local fields, $h_i = 0$.

While problems with local fields or large ferromagnetic structure (e.g. embedded problems) could benefit from specific analysis, we expect that the general results and arguments presented will be generalizable to a large range of problem sets.

A. Forward annealing with a pause

We consider the following simple adaptation to the standard annealing schedule. Allow the system to run as normal to some (re-scaled) time $s_p \in [0, 1]$, upon which we pause the system for time $t_p \in [0, 2000] \mu s$, after which we continue the evolution as per normal.

Fig. 5 shows that this pause dramatically affects the samples returned from the annealer. While Fig. 5 is for one instance, almost all instances we tested exhibit this behavior, including a strong peak in the success probability when a pause is inserted into the regular annealing schedule within a narrow band of values of $s_p$. Fig. 5 shows that the corresponding average energy returned is also significantly reduced. We define the ‘optimal pause point’, $s_p^{opt}$, as the point in the anneal for which a pause returns the lowest average energy returned from many samples [26] (just after $s_p = 0.4$ in this example).

Fig. 6 shows that the longer the pause, the greater the increase in the success probability. Here, we see that the success probability, for a pause at re-scaled time $s_p = 0.44$, increases from the baseline ($\approx 0.01\%$) to over 10% for pause lengths longer than around 500 $\mu$s, and approaches 20% as the pause length approaches 2ms (the longest allowable pause length on the D-Wave machine), although saturating around 1ms (in the logarithmic regime). That is, an increase of around three orders of magnitude. This behavior gives us new insight into the time-scales involved in these annealers. It shows that even a 10 $\mu$s pause (inserted within a default schedule with $t_a = 1 \mu s$) can dramatically effect the nature of the samples returned from the annealer.

These observations are consistent with the thermalization picture mentioned in the previous section, and the cartoon in Fig. 4; we attribute the purple region in Fig. 4 to the region where the huge spike in success probability is observed, since the system can effectively relax back to the low lying energy levels on a time-scale comparable with the pause length. After this (e.g. the blue region in Fig. 4), the effect is much weaker (dropping off exponentially) as the relaxation time scale increases (notice in Fig. 5 that late in the anneal, the relative increase in success probability is much less, or non-existent, as compared to during the region around $s_p = 0.4$).

We observe similar phenomena for the second problem class we study (with $J_{ij} \in [-1, 1]$), as in Figs. 7,8. In
FIG. 5. Forward annealing with a pause for a single 783 qubit (planted-solution) problem instance \( (I_{783}) \). The top figure shows the success probability with respect to pause length \( t_p \), and the location of the pause \( s_p \). The total evolution time (aside from the pause) is \( 1 \mu s \). The corresponding bottom figure shows the average energy (in arbitrary units) returned by the annealer. Each data point is averaged from 10000 anneals with 5 different choice of gauge. In the absence of a pause, \( P_0 \approx 10^{-4} \).

In these figures we show the effect of changing the pause length, and the total anneal time respectively.

An effect we observe upon increasing the pause length is that the width of the peak increases, as shown in Fig. 7. Notice that in this figure all curves start to show an increase in success probability at the same pause point \( s_p \) (just after 0.4), but come back to the baseline probability at later points for longer pause lengths. That is, the region of interest is slightly extended to the right. This also fits in with the model discussed in Sect. 1C and the cartoon picture Fig. 4, where increasing \( t_p \) increases the size of the purple region by extending it to the right (i.e. the region where \( t_H < t_r \leq t_p \)). The location of the peak \( s_p^{\text{opt}} \) we posit to be around the point \( t_r \approx t_p \), the last point in the anneal for which thermalization can effectively occur during a pause of length \( t_p \). Indeed we experimentally observe (in Fig. 7) that increasing the pause length shifts the peak to later in the anneal (and also increases in size \( P_0 \) in accordance with this picture [27]).

If one instead increases the anneal time (hence \( t_H \)), the peak narrows (and flattens), and eventually disappears, as observed in Fig. 8. Note, in accordance with Fig. 4, the location of \( s_p^{\text{opt}} \) does not change upon increasing \( t_a \) (since this should reduce the size of the purple region from the left). We also show a corresponding heat map of this effect in Appendix D (Fig. 26).

It is remarkable that the peak is extremely well defined, occurs in such a concentrated region, and exists for almost all problems we studied (the only exception being some small problem instances, which we discuss below). For problems of the planted-solution type, there seems to be little dependence on problem size for the position of this peak. Fig. 9 plots the optimal pause point, \( s_p^{\text{opt}} \), which does not vary much with problem size and, in addition, the deviation (i.e., the error bars in the figure) in the samples appears more or less constant. For problems generated with \( J_{ij} \in [-1,1] \) (uniformly random), we see a mild effect with increasing problem size, in which the optimal pause point seems to decrease, and concentrate in location (i.e. the error bars in the figure are decreasing with problem size). This effect would presumably saturate with large enough \( N \) (note, in the figure, SL=16 is the largest possible problem size available).

The simple observations demonstrated here show that one may be able to design more efficient annealing schedules by annealing very quickly, and pausing for a rela-
FIG. 7. Effect of changing the pause length for a 12-qubit problem instance ($I_{12}$). Each data point is from 10000 annealing runs using 5 different gauges. The anneal time $t_a = 1\mu s$ for all data sets shown.

FIG. 8. Effect of changing the anneal time for $I_{12}$. Each data point is from 10000 annealing runs using 5 different gauges. The pause length $t_p = 100\mu s$ for all data sets shown.

tively short time, as compared to running the default annealing schedule for a long time. Moreover in Fig. 10, we see the width of the peak only depends very weakly (or not at all) on the problem size; this suggests that for most problems, regardless of size, there is a fairly large window in which one can pause and observe an increase in success probability, potentially by orders of magnitude, see Fig. 11.

B. Reverse annealing with a pause

Before proceeding with a statistical analysis we briefly present some relevant results using the reverse annealing protocol, with a pause, the general protocol of which is demonstrated graphically in Fig. 3. This allows us to identify some of the key regions during an anneal, which, as explained above, depend on the ratios of the various energy scales involved and associated time-scales.

We show some of our findings in Fig. 12 where we identify 4 regions of interest. 1) $s_p < s_{gap}$. The system has been evolved (from $s = 1$) past the minimum gap, and been paused at a point where $Q > O(1)$, allowing for mixing between energy levels in the computational basis. There is no memory of the initial configuration. 2) In the region just after the minimum gap, up to around $s_{opt}^p$, where the lowest energy solutions are found, and corresponding to the purple region in Fig. 4. Here there is no memory of the initial state, and no clear difference between forward and reverse annealing. We expect thermalization is able to occur effectively on timescales comparable with $t_p$, i.e., the transition rates between energy levels $\Gamma_{ij} \geq 1/t_p$. 3) After $s_{opt}^p$, where there is a clear difference between forward annealing and reverse annealing, there is ‘memory’ of the initial configuration. Thus the state returned by the annealer at $s = 1$ depends heavily on the system state at the pause point $s_p$, suggesting different time-scales and transition rates are important here. In this region, as $Q \to 0$ and $\langle E_i|\sigma^z|E_j \rangle \to 0$, the $g_{x,y}$ couplings may play more of a role, leading to qualitatively different thermalization mechanisms and timescales. Here some transition rates $\Gamma_{ij}$ may be comparable
FIG. 10. The width of the peak on a graph of $|\langle E \rangle|$ Vs. $s_p$, as a function of problem size. The ‘full-width-at-half-maximum’ (FWHM) is the width of the peak in the energy curve $|\langle E \rangle|$ as a function of $s_p$, at $(|\langle E(s_{opt}^p) \rangle| + |E_{BG}|)/2$ where $E_{BG}$ is the background average energy (i.e., the average energy returned from the annealer in the absence of a pause), and $E(s_{opt}^p)$ the (mean) energy returned by the annealer at the optimal pause point. Note, modulus is used since all energies observed negative. The problems (same as in Fig. 9) were generated on a square subgraph of the chimera with ‘side-length’ $SL$, consisting of $SL \times SL$ unit cells each containing 8 qubits (e.g. see Fig. 2 in Ref. [11]). Each SL shown [4, 8, 12, 16] corresponds to (taking account for dead qubits) $N = [127, 507, 1141, 2031]$ respectively. Each data point shown is an average over (at least) 50 instances. Error bars represent the standard deviation. Each instance (for each $s_p$ tested) is averaged from 10000 anneals with 5 different choice of gauge, with $t_a = 1 \mu$s (not including the pause time), and $t_p = 100 \mu$s.

to $1/t_p$, whereas others much less. 4) Very late in the anneal, with $Q \ll C \ll 1$, almost no dynamics occur (the state returned from the annealer is almost always the same as the one initialized), i.e. $\Gamma_{ij} \ll 1/t_p$.

We mention that these general observations seem to be fairly generic, and not specific to this particular example. With this in mind, we proceed with a statistical analysis, demonstrating to what extent the picture outlined in Fig. 4 holds.

C. Correlation with the minimum gap

Typical folklore of (open system) quantum annealing dictates that around the location of the minimum gap, thermal excitations from the ground state to excited energy levels may occur, and that after the gap, thermal relaxation will allow some of the excited population to fall back to the ground state [28] (of course, this is heavily dependent on the nature of the minimum gap, and hence on $H_p$ itself, as well as the temperature and annealing schedule). This general idea is also demonstrated in Fig. 4. This framework would suggest that a pause in the

FIG. 11. For the planted problems of Fig. 9 (50 instances per side-length), we plot the success probability under the default annealing schedule (with $t_a = 1 \mu$s) $P_0$ as compared to the success probability for an anneal with pause ($t_p = 100 \mu$s) at the optimal pause point, $P_0(s_{opt}^p)$. We see typically orders of magnitude improvement for the hard problems. Note, the problems which are plotted vertically on the y-axis have $P_0 = 0$ (i.e. were not solved once over all anneals). Note, some problems which were not solved once, even under the pause, are not included.

FIG. 12. Reverse annealing with pause at $s_p$ (solid lines), for a four different initial configurations for a 12-qubit problem $Z_{12}$. We plot the average energy (arbitrary units) returned from 5000 anneals, evolved at rate $d^2s/dt^2 = 1 \mu$s$^{-1}$, and $t_p = 100 \mu$s. We consider ground and first excited state configurations, as well as two highly excited energy levels. The energy level $E_i$ is indicated on the right hand side. We also show the corresponding forward anneal curve (black-dash line). This problem has a minimum gap at $s = 0.44$ indicated in the figure. Note a sample of the spectrum for this problem is shown in Fig. 22 in Appendix A.
formly random) and of size 12 qubits. These problems have
$J_{ij} \in [-1,1]$ (uniformly random) and $h_i = 0$. We divided the data into two
4. We fixed the pause length to $t_p = 1000\mu s$, and total anneal time (excluding the pause)
to $T_a = 1\mu s$. Data from the annealer is averaged over 10000
annealing schedule some (problem dependent) time after
the minimum gap may lead to an increase in the success probability (that is, the population in the ground state
at time $s = 1$).

Working with 12-qubit problems with $J_{ij} \in [-1,1]$ (uniformly random), we indeed find such a correlation
between the location of the minimum gap, and the optimal
pause point, $s_{\text{opt}}^p$, where for over 90 of the 100 problems
tested the best place to pause is after the minimum gap. This is demonstrated in Fig. 13, where on average
$s_{\text{opt}}^p \approx s_{\text{gap}} + 0.14$.

We comment briefly on the few outliers (e.g. with
$s_{\text{gap}} < s_{\text{opt}}^p$, or not in the main cluster of points) in the data set. For some of these 12-qubit problems, they are solved almost 100% of the time by the D-Wave annealer (i.e. they are extremely easy optimization problems). These problems have that large minimum gaps
$\Delta_{\text{min}} > 1\text{GHz}$, and we indicate them in red in the plot (also see Fig. 25 in Appendix D). For these instances, we typically do not observe a well defined optimal pause point; since the gap is so large for all $s$, we expect very little thermal excitation to occur at all, hence pausing has little effect. We see these red points have a fairly random spread in the $s_{\text{opt}}^p$-axis.

The second set of outliers are (some of the) instances which have minimum gaps relatively late in the anneal.

We observe these instances do not have well defined optimal pause points, and expect this is due to quirks of their individual spectra (one such example is shown in Fig. 27 of Appendix D). In particular when the minimum gap occurs late in the anneal (e.g. after the point when $Q < 0.1$), either the transition time scale $t_r$ may already be too large for effective thermalization to occur during a pause (since the $\sigma^x$ matrix elements driving the transitions in Eq. (2), governed by $Q$, are negligible), or the gap doesn’t open up enough before the end of the anneal to transfer enough population out of the excited states.

It is interesting to note that the observation of instances without well defined optimal pause points appears to be a small size effect, since all of the (both planted, and uniformly random) problems tested in Fig. 9 (which all had over 100 qubits) had well defined optimal pause points, i.e. all exhibited a well defined minima in the energy as a function of pause point (and peak in the success probability as a function of pause point, for the planted problems).

Nevertheless, the overall trend is clear, with the majority of problem instances exhibiting an optimal pause point in a narrow region shortly after the location of the minimum gap.

We similarly study the same problems where we re-scale the problem Hamiltonian by a constant factor (2,4,8). This has two effects: 1) it shifts the location of the minimum gap to later in the anneal, and it also reduces the size of the minimum gap (as an explicit example, see Fig. 28 in Appendix D). We indeed see that correspondingly, the location of the optimal pause point shifts to later in the anneal (see inset of Fig. 14). We show this explicitly for a single problem in Fig. 29 in Appendix D.

Interestingly, we also observe that the location of $s_{\text{opt}}^p$ concentrates (thus becoming less correlated with $s_{\text{gap}}$) upon reducing the energy range of the problem; notice how in Fig. 14, the purple points ($H_{\text{opt}}/8$) are almost perfectly aligned close to $s_{\text{opt}}^p = 0.8$. We also see this by noting that the error bars (standard deviation) in the $s_{\text{opt}}^p$-axis decrease (inset of figure).

We explain this behavior by pointing out that by dividing $H_p$ by a large enough factor, $\beta \omega_{01} (s) < 1$ for $s > s_{\text{gap}}$
where $\omega_{01} (s) := E_1 (s) - E_0 (s)$ is the gap between the ground and first excited state, and $\beta$ the inverse temperature of the annealer. This implies the system should be able to effectively thermalize until very late in the anneal, until the matrix elements in Eq. (2) become small enough (determined by $Q$ being small enough). This picture means the start of the region when the dynamics become frozen (purple region in Fig. 4) is not determined so much by the problem itself (i.e. the exact spectrum as a function of $s$), but the annealing schedule (i.e. $Q(s)$). Thus different problems may exhibit very similar optimal pause points.

It would be worth while to explore this in more detail to confirm this hypothesis.
D. Quantum Boltzmann distribution

For a set of 10 problem instances of size 12-qubits $T_{12}^{0-9}$ (each with well defined optimal pause points, with $\Delta_{\text{min}} < 1\text{GHz}$, $Q(s_{\text{gap}}) > 0.1$) with $J_{ij} \in [-1, 1]$ (uniformly random), we compare the returned statistics to the instantaneous quantum Boltzmann distribution $\rho \sim \exp(-\beta H(s))$ (projected to the $z$-eigenbasis), for various choices of $\beta$; we vary the temperature $T$ from $\frac{1}{4}T_{\text{DW}}$ to $4T_{\text{DW}}$, in increments of $\frac{1}{4}T_{\text{DW}}$ (where $T_{\text{DW}} = 12.1\text{mK}$ is the operating temperature of the annealer). We outline these calculations in Appendix B.

We study these problems, with a very long pause length of $t_p = 1000\mu s$ to allow enough time to thermalize, and run with short anneal time (excluding pause time) $t_a = 1\mu s$, i.e. the quickest possible rate $\frac{d^2}{dt^2}$, so that we can try to isolate the effect of the pause by ‘quenching’ the system.

An example of this analysis for a single instance is shown in Fig. 15, however we note the pattern looks much the same for all of the instances studied (see Fig. 16). Here, we focus on the distribution returned from the annealer with a pause at the optimal pause point $s_{p}^{\text{opt}}$, and compare this to a distribution of the form $\exp(-\beta H(s))$. It is interesting to note that we do indeed seem to observe a correspondence between the projected quantum Boltzmann distribution at the optimal pause point, and the data sampled from the experimental device.

Having said this however, we observe that the experimental distribution is best described by a hotter Boltzmann distribution, at a later point in the anneal than the optimal pause point. In particular for these problems the optimal parameters $(s^*, T^*)$ such that $D_{\text{KL}}$ is minimized, correspond to $s^* = 0.78 \pm 0.10$ and $T^* = 26.1 \pm 8.8\text{mK}$ (and up to 4 times the physical temperature). Moreover, $s^* - s_{p}^{\text{opt}} = 0.21 \pm 0.11$ (i.e. significantly later in the anneal than the optimal pause point). At values of $s^*$ this late in the anneal (with $Q(s^*) \approx 10^{-3}$), the distribution is indeed effectively a classical Boltzmann distribution (of $H_p$); that is, $\exp(-\beta H_p)$, where $\beta$ is an effective inverse temperature (one which is typically hotter than $T_{\text{DW}}$).

This result is somewhat confusing. For one, the temperatures seem to vary wildly between instances as seen in Fig. 16, and moreover, it suggests that non-trivial dynamics can occur well past the optimal pause point. Since we expect the region around the optimal pause point to correspond approximately to when the dynamics are diminished to the point where the system is frozen (i.e. the region where the system time-scale is short compared to the thermal time-scale, and quantum fluctuations $Q$ are small), one may expect to see a closer match between $s^*$ and $s_{p}^{\text{opt}}$.

We conjecture that after the optimal pause point non-trivial dynamics do indeed still occur. The intermediate pause helps the D-Wave distribution equilibrate to the instantaneous thermal distribution, and after this, although the thermal transition rate is too small to thermalize effectively (even with a pause), some dynamics will inevitably occur. Indeed, since for these problems, the optimal pause point occurs around $s_{p}^{\text{opt}} = 0.55$, where $Q \approx 0.1$, it is possible that there are even still some internal (quantum) dynamics driven by $Q$. Therefore the distribution one eventually measures may not quite be a projection of a Boltzmann distribution at a well defined $(s, T)$.

We partly validate this picture in Fig. 17 comparing the D-Wave distribution of a single instance to the optimal found over all $(s, T)$ in $\exp(-\beta H(s))$. This problem fits best to a Boltzmann distribution with optimal values $(s^*, T^*) = (0.76, 18.5\text{mK})$. We plot on a logarithmic scale to show the similarity to a classical Boltzmann distribution of $H_p$, for which $\ln \frac{T}{2} = -\beta E_i - \ln Z$ (i.e. a straight line on this graph). This late in the anneal we expect the Boltzmann distribution to be approximately of the form $\exp(-\beta H_p)$ for some appropriate $\beta$, since $Q(s^*) < 10^{-2}$.

We notice that indeed, both the experimental data and the computed Boltzmann distribution seem to fit reasonably well to a linear fit (indicating classical thermalization is occurring to some extent), but also mention it is not clear whether the two distributions correspond to one and the same; there are clearly some large divergences (the $y$ axis is a logarithmic scale).

It is also interesting to note that in the absence of a pause we do not see any clear correspondence between the D-Wave distribution and a Boltzmann distribution. For example, for the distribution returned from an anneal with pause at $s_{p}^{\text{opt}}$, the minimum KL divergence is $D_{\text{KL}}\min = 0.016 \pm 0.015$ and $D_{\text{KL}}(s_{p}^{\text{opt}}, T_{\text{DW}}) =$
FIG. 15. KL divergence $D_{KL}$ between data from the annealer $P_{DW}$ and the Boltzmann distribution $P_{QBM}$ (projected into the computational basis) for various choices of $(s,T)$, for a single 12-qubit instance ($I_{12}$). The D-Wave data is sampled from a pause of length $t_p = 1000\mu s$ at $s_{\text{opt}}$, with $t_a = 1\mu s$ (from 10000 anneals and 10 choices of gauge). We indicate in the plot three key parameters; the physical temperature $T_{DW}=12.1\text{mK}$, the location of the minimum gap $s_{\text{gap}}$, and the optimal pause point $s_{\text{opt}}$. The white diamond corresponds to the minimum value of $D_{KL}$ over all $(s,T)$, and is equal to $D_{KL}^{\text{min}}=0.01$ bits of information. Note, to be able to distinguish the features in the plot, we set the upper limit on the plot to be $D_{KL}=0.2$ (any value above this is mapped to this color).

FIG. 16. For the 10 problems described in the main text ($I_{12}^{0-9}$), we plot the values $(s^*,T^*)$ (relative to $s_{\text{opt}}$) which correspond to the minimum value of $D_{KL}$ over all choices of $(s,T)$ tested. We see the same trend for all of the problems, as observed directly in Fig. 15, where larger $s^*$ implies larger $T^*$. Note in the plot, two of the data points lie on top of each other. The mean optimal KL-divergence found for these problems was $D_{KL}^{\text{min}}=0.016 \pm 0.015$. Note, $T_{DW}=12.1 \pm 1.4\text{mK}$.

0.076 \pm 0.065). However, performing the same analysis with an anneal with no pause, the values vary wildly, with $D_{KL}^{\text{min}}=0.19 \pm 0.15$. That is (over the range of $(s,T)$ for which we computed $\exp(-\beta H(s))$) there is typically no good choice of $(s,T)$, and it is not clear what the distribution is.

If the system is not able to thermalize appropriately during the anneal (e.g. because the anneal time $t_a$ is too quick), there is no expectation for the D-Wave distribution to be close to any Boltzmann distribution.

With this in mind, though we have provided evidence suggesting thermalization is occurring to some extent in these problems, more work is required to understand precisely the distribution one is sampling from at the optimal pause point. In particular, we would like to better understand why the fitting temperature seems to vary so much between these instances, and why the dynamics seem to occur so long after the optimal pause point. The main constraint in our experiments prohibiting us to probe these details further is the maximum annealing rate $\frac{ds}{dt}$ which is limited to $1\mu s^{-1}$ on the present annealer. That is, even though we hope to be approximately quenching the system from after the optimal pause point (i.e. measuring in the middle of the anneal), in reality non-trivial internal dynamics, driven by $Q$, may still occur before late in the anneal.

We provide some more intriguing evidence in the next section, where we focus on a set of (large-scale) problem...
instances which indeed seem to exhibit classical thermalization (i.e. thermalization to a Boltzmann distribution of $H_p$).

E. Classical Boltzmann distribution

The extent to which annealers sample from a classical Boltzmann distribution at some point $s^*$ late in the anneal is a hotly contested issue [5–8, 11]. Sampling from a Boltzmann distribution is NP-hard, so annealers would not be expected to efficiently solve this problem across the board, but they could have advantage over the best classical methods. Quantum computing is known to have advantages over classical computing for sampling from certain distributions [29, 30], including Gibbs distributions [31], but whether quantum annealing has an advantage remains an open question. If problems for which machine learning is applicable (e.g. in the restricted Boltzmann machine paradigm) freeze-out at a point late in the anneal, when $Q \ll 1$, then annealers may have an advantage over classical samplers [6, 7, 9].

With the advent of a new entropic sampling technique based on population annealing [10], we were able to accurately estimate the degeneracies for 225 planted-solution instances containing 501 qubits (that is the estimated ground and first excited state degeneracies are within 5% of the known values found by planting). For more information on these techniques see Refs. [10, 11], and Appendix C. Due to the large size of these problems, we are of course not able to compute the Boltzmann distribution of the full Hamiltonian $H(s)$ as we did in the previous section.

However, having accurate values for the degeneracies allows us to calculate the classical (problem Hamiltonian) Boltzmann distribution $\rho \sim \exp(\beta H_p)$, where $\beta$ is an instance-dependent effective inverse temperature, i.e., a fitting parameter, which depends on the physical temperature, and the strength problem Hamiltonian $B(s)$ (and in principle anything else effecting the distribution returned from the annealer such as various noise sources).

If the distribution returned from the D-Wave machine is indeed a classical Boltzmann distribution at freeze-out point $s^*$ late in the anneal (when $Q(s^*) \ll 1$, then one would expect (ignoring any other noise sources) to find $\beta = \beta_B(s^*)/J_{\max}$, where $\beta = 1/k_B T$ is the physical inverse temperature, $B(s^*)$ is the problem Hamiltonian strength at the freeze-out point, and $J_{\max} = \max |J_{ij}|$ is a normalization parameter (since the $J_{ij}$ programmed into the quantum annealer are restricted to the range $[-1, 1]$).

We make two key observations. 1) all of these problems tested exhibit a strong peak in the success probability in a fairly narrow region $s_{p, opt}^* \in [0.35, 0.46]$ (i.e., much less varied than the 12-qubit instances studied above). 2) The data returned from the annealer, for all of these problems, matches closely to a classical Boltzmann distribution for $H_p$, but at a higher temperature than the operating temperature of the annealer (at least 1.5 times higher). This is in accordance with the results of Ref. [11] where calculated freeze-out points for most large problems were very early in the annealing schedule (equivalent to a higher than expected temperature), although in this work, a pause during the anneal to more directly study thermalization was not available. We demonstrate these points below.

First consider Fig. 18 where for a single instance we plot $\ln \frac{p_i}{p_i}$ against $E_i$, where $p_i$ is the probability of observing a configuration with energy $E_i$, and $g_i$ is the degeneracy of that energy level. One can see the data returned from the annealer is nearly indistinguishable from a linear fit (for all problems, and all pause points $s_p$, we find the $R^2$ (coefficient of determination) value is greater than 0.97, and up to 0.9999). That is, the data from annealer seems to fit to $p_i = \frac{1}{Z} e^{-\beta E_i}$, for some constants $Z$, and $\beta$ (which can be determined by least-squares fitting).

Though the results are clear, the correct interpretation of them is not. For example, if we obtain the effective inverse temperature of the distribution $\beta$ from the least squares fitting, and set it equal to $\tilde{\beta} = \beta_B(s^*)/J_{\max}$, with knowledge of $\beta = 1/k_B T$, and $J_{\max}$, we can calculate $B(s^*)$. If one does this however, the value returned cor-
responds to an extremely early point during the anneal, even earlier than \( s_{\text{opt}} \) (e.g. with \( Q \approx 1 \), or equivalently \( s \approx 0.35 \)). If one however assumes the thermalization picture presented in Sect. 1C, which suggests the dynamics should freeze when the relaxation time scale is longer than the system time scale, i.e. approximately around the optimal pause point, \( s_{\text{opt}} = 0.42 \pm 0.01 \) for these problems, the temperature required for the fit is \( > 1.5 \) times higher than the physical temperature \( T = 19.8 \pm 1.1 \text{mK} \) (compared to \( T_{\text{DW}} = 12.1 \pm 1.4 \text{mK} \)).

It is however not clear whether \( \exp(-\beta H(s^*)) \) with \( s^* = 0.42 \) and \( Q(s^*) \approx 0.5 \) would indeed correspond to a classical Boltzmann distribution (of \( H_p \)) since the off diagonal driver is still relatively strong in magnitude. Indeed, this is a somewhat similar result as from the previous section where we observed the optimal parameter value for \( s \) was in fact slightly after \( s_{\text{opt}} \) (and \( T \) larger than the physical temperature). If there are in-fact still dynamics after \( s_{\text{opt}} \), the dynamics will be frozen somewhat later in the anneal (when \( Q(s) \) is smaller), and the associated temperature of the fit will be larger. We discuss some implications of this in the next section. For now we compare the samples from the optimal pause point to those from outside of it.

In Fig. 19 we plot the \( R^2 \) value found by the least squares fitting for a typical instance as a function of pause point \( s_p \). We see that the peak corresponds closely to the optimal pause point under the pause. Moreover, we see a very similar trend for all of the problems we tested, with the pause point for which the largest \( R^2 \) value is observed differing by at most 3% of the annealing schedule from the optimal pause point: \( s_{\text{opt}}^{\text{max}} = s_{\text{opt}} \pm 0.03 \). This indicates that the data returned from a pause at this critical point, fits better to a classical Boltzmann distribution, as compared to the rest of the data (or indeed, from the distribution returned in the absence of a pause in the schedule). If indeed the problems are thermalizing to a classical Boltzmann distribution, this work shows that by pausing the anneal at a particular (instance-dependent) point allows a more complete thermalization to occur. This result is similar to that found in the previous section.

We performed a similar analysis for three other problem sizes (\( N = 31, 125, 282 \) qubits), and find that increasing the problem size in general increases the mean \( R^2 \) value for a fit to a classical Boltzmann distribution. For \( N = 31, 125, 282, 501 \), the corresponding values are \( \langle R^2 \rangle = 0.911, 0.994, 0.995, 0.997 \), where the average (median) is over all instances and all pause points \( s_p \) tested. Moreover, the correlation between \( s_{\text{opt}} \) and \( s_{\text{opt}}^{\text{max}} \) seems to also increase with problem size, as demonstrated in Fig. 20, which shows the variation between different instances decreases with problem size, and seems to suggest that \( s_{\text{opt}} \approx s_{\text{opt}}^{\text{max}} \), for large \( N \) (i.e., the optimal pause point and the pause location for which the best fit to a Boltzmann distribution is observed, coincide for large problems).
III. SUMMARY AND OUTLOOK

Our work demonstrates that even enabling simple adaptations of the default annealing schedule, such as pausing, can provide orders of magnitude improvements in performance. For the two classes of problems we studied, we found a critical region for which if one pauses, even for a relatively short time (say 10μs), a drastically different distribution of solutions is returned. In particular, annealing with a pause in this region more effectively samples low lying energy states in this region, resulting in a larger probability of success. The best place to pause is around 10-15% of the total anneal time after the minimum gap (for the problem class we studied). This effect does not make sense in a closed-system scenario, as discussed in Appendix A, but can be explained, at least qualitatively, in terms of open system dynamics, particularly thermalization. The qualitative picture we discussed suggests that after the minimum gap – when thermal excitations may allow a significant fraction of the population to leave the ground state – population can begin to thermally relax back into the ground state. This picture also explains the sharp-peaked nature of our observations; if one pauses just a little too late, since the transition rates depend exponentially on the size of the instantaneous energy gaps they quickly drop off, and the pause length becomes too small (relative to the instantaneous relaxation time) for effective thermalization to occur. The exact behavior depends heavily on the spectrum of each individual instance, since this determines the transition rates.

Our results provide positive evidence for the Boltzmann nature of the distributions returned from the annealer, even for the majority of problems for which, as was shown in Ref. [11], a sensible freeze-out point does not exist. To obtain further insight into the nature of the distributions at the end of the anneal, we performed two studies. On small (12-qubit) problems for which we are able to compute the quantum Boltzmann distribution for every point in the anneal, we compare the final distribution to the projected quantum Boltzmann distribution. For larger problems, it is not feasible to compute the quantum Boltzmann distributions throughout the anneal, but with the aid of recent entropic sampling techniques that enable accurate estimation of the eigenspectrum degeneracies for a class of planted solution problems, we were able to fit the final distribution, for multiple pause locations, to a classical Boltzmann distribution for \( H_p \) with the effective temperature as a fitting parameter.

The first study showed that the best performance occurs when the pause takes place after the minimum gap, confirming our qualitative picture. Further, the fit between the projected quantum Boltzmann distribution and the final distribution is poor except when the pause is in the region shortly after the gap, strongly suggesting that the pause contributes significantly to thermalization. The best fit between the final distribution and the projected quantum Boltzmann distribution occurs somewhat after this pause point, and was much higher than the physical temperature, and the temperature fluctuated wildly between instances. Moreover, the fluctuating temperatures do not seem consistent with the physical temperature fluctuations on the annealer. It is unclear from our picture as to where one would expect the best fit to be because there may be significant dynamics after the optimal pause point. Further, there may be discrepancies between the computed quantum Boltzmann distribution and the distribution that would be predicted if we had better knowledge of the device. The computed effective temperature depends on the device temperature, which is sampled only coarsely in time, and may not be the temperature at the qubits, and may also fluctuate within a single anneal. Control errors on the \( J_{ij} \) can also have significant effect on the distribution [32]. Future work with more flexible and instrumented annealers, as well as theoretical advances, will further deepen our understanding open system dynamics and quantum annealing.

The second study showed that the best fit between the final distribution and a classical Boltzmann distribution for \( H_p \) occurs, for all instances, when the pause is at the optimal pause point, indicating these samples are thermalizing more completely, and again confirming our qualitative picture. In this case, an excellent fit between a classical Boltzmann distribution for \( H_p \) and the final distribution occurs at all points, and even in cases in which no pause has been inserted. Our results further suggest that the larger a problem is, the more likely it is to have a good fit to a classical Boltzmann distribution. By varying the pause point, one can effectively vary the temperature at which one samples from the classical Boltzmann distribution, with potential implications for machine learning, such as the use of quantum annealing in restricted Boltzmann machines. The fits are obtained with effective temperature as a free parameter. We find that generally the effective temperature is substantially higher than predicted. As with the small problem study, discrepancies between the device temperature and the qubit temperature, fluctuations in this temperature during an anneal, and control errors masquerading as higher temperatures may all contribute to a higher effective temperature. While the device temperature is sampled only infrequently, the fluctuations in fitted temperature did fairly consistently track those of the actual device, unlike in the small problem study. A further difficulty in interpreting this data is that the optimal pause point seems slightly too early in the anneal to observe a classical Boltzmann distribution. Again, hardware and theory advances are needed to fully clarify this picture.

An obvious next step would be to investigate the effect of pausing on other problem classes, particularly embedded problems related to applications. Key questions include the extent to which pausing improves performance in other problem classes, and the robustness of the region in which pausing is effective across instances within each class and as the size of the problems grow. A natural
question to ask is the extent to which yet more flexibility in the annealing schedule can provide yet greater improvements in performance. A significant challenge to the field is to provide more theory guidance, beyond the qualitative picture presented here, in order to (i) better explain the results we presented, (ii) suggest which new features would be most effective to add in the next generations of quantum annealers, and (iii) guide the design of effective annealing schedules on current and future generations of these devices. Early challenges for such a theory would be to predict the location and width of the effective pause regime, and particularly how they scale with problem size, and to characterize the output distributions, particularly the effective temperature of the best fit Boltzmann distribution for $H_p$, deviations for Boltzmann, and scaling with problem size.

Based on the study we present here, useful features of future quantum annealers would include both a faster quench and more accurate temperature data. On the D-Wave 2000Q, no part of the schedule can be traversed faster than $\frac{ds}{dt} = 1\, \mu s^{-1}$. We would like to more precisely understand the distribution at the optimal pause point. To do so, one would need to be able to more effectively quench the system. Enabling faster traversal of the schedule, particularly in the 3rd and 4th regions of the anneal (see Fig. 4), would enable experiments giving greater insights into the distributions during the anneal than are possible currently. An alternate means for performing a fast quench or the addition of probes mid anneal would also provide insight. With regard to the temperature, it would be helpful to have further insight into the extent to which (i) the temperature at the qubits differs from that of the measured device temperature, (ii) the temperature changes during the course of the anneal, and (iii) control errors, such as deviations in the values of the $J_{ij}$ on the device from the intended values. While deep probing of the temperature is experimentally challenging, lighter probing should be possible, and even access to finer-grained temperature data than the current rate of once every few hours would help fill out the picture.

The qualitative picture we give to explain our results suggests that similar behaviour will be found in problem classes more closely tied to applications, both in machine learning and optimization. The relative robustness across instances within a problem class of the location and width of the region in the annealing schedule for which a pause substantially improve results suggests that good heuristics for the pause length and location may be derivable from empirical evaluation of a few instances within a problem class. While the region in which a pause is effective is only a fraction of the anneal schedule, that region is substantially wider than that of the minimum gap, suggesting both greater robustness and greater ease in finding effective locations in which to pause or slow down than in closed system adiabatic quantum computing. This robustness also suggests that it may be more feasible to find effective adaptive methods, making use of judicious measurements in the course of a single anneal to the adjust the schedule, than in closed system adiabatic quantum computing. More generally, a deeper open systems understanding would give insight into the design of both annealing schedules and quantum hardware, from annealers to universal quantum computers.

IV. DATA ACQUISITION

For all instances labeled as $\mathcal{I}_N$ (where $N$ is the qubit number, and $s$ a serial number when applicable), we provide the problem instance itself as part of the ancillary files associated with this article. Any other problem instances (and data) available upon request.

ACKNOWLEDGMENTS

We thank Lev Barash for computing the degeneracies of the 500 qubit problems in Sect. II E. E.G.R. and D.V. would like to acknowledge support from the NASA Transformative Aeronautic Concepts program and the NASA Ames Research Center. D.V. was supported by NASA Academic Mission Services (NAMS), contract number NNA16BD14C, and J.M. by the USRA Feynman Quantum Academy under NAMS. E.G.R. and D.V. were also supported in part by the AFRL Information Directorate under grant F4HBKC4162G0001 and the Office of the Director of National Intelligence (ODNI) and the Intelligence Advanced Research Projects Activity (IARPA), via IAA 145483. I.H. was partially supported by the Office of the Director of National Intelligence (ODNI), Intelligence Advanced Research Projects Activity (IARPA), via the U.S. Army Research Office contract W911NF-17-C-0050. The views and conclusions contained herein are those of the authors and should not be interpreted as necessarily representing the official policies or endorsements, either expressed or implied, of ODNI, IARPA, AFRL, or the U.S. Government. The U.S. Government is authorized to reproduce and distribute reprints for Governmental purpose notwithstanding any copyright annotation thereon.

[1] T. Albash and D. A. Lidar, “Demonstration of a Scaling Advantage for a Quantum Annealer over Simulated Annealing,” Phys. Rev. X 8, 031016 (2018).

[2] V. S. Denchev, S. Boixo, S. V. Isakov, N. Ding, R. Babush, V. Smelyanskiy, J. Martinis, and H. Neven, “What is the Computational Value of Finite-Range Tunneling?”
[3] T. F. Rønnow, Z. Wang, J. Job, S. Boixo, S. V. Isakov, D. Wecker, J. M. Martinis, D. A. Lidar, and M. Troyer, “Defining and detecting quantum speedup,” Science 345, 420 (2014).

[4] S. Mandrà, Z. Zhu, W. Wang, A. Perdomo-Ortiz, and H. G. Katzgraber, “Strengths and weaknesses of weak-strong cluster problems: A detailed overview of state-of-the-art classical heuristics versus quantum approaches,” Phys. Rev. A 94, 022337 (2016).

[5] M. H. Amin, “Searching for quantum speedup in quasistatic quantum annealers,” Phys. Rev. A 92, 052323 (2015).

[6] M. H. Amin, E. Andriyash, J. Rolfe, B. Kulchytskyy, and R. Melko, “Quantum Boltzmann Machine,” Phys. Rev. X 8, 021050 (2018).

[7] M. Benedetti, J. Realpe-Gómez, R. Biswas, and A. Perdomo-Ortiz, “Estimation of effective temperatures in quantum annealers for sampling applications: A case study with possible applications in deep learning,” Phys. Rev. A 94, 022308 (2016).

[8] B. H. Zhang, G. Wagenbreth, V. Martin-Mayor, and I. Hen, “Advantages of Unfair Quantum Ground-State Sampling,” Sci. Rep. 7, 1041 (2017).

[9] S. H. Adachi and M. P. Henderson, “Application of Quantum Annealing to Training of Deep Neural Networks,” arXiv:1510.06356 (2015).

[10] L. Barash, J. Marshall, M. Weigel, and I. Hen, “Estimating the Density of States of Frustrated Spin Systems,” arXiv:1808.04340 (2018).

[11] J. Marshall, E. G. Riedel, and I. Hen, “Thermalization, freeze-out, and noise: Deciphering experimental quantum annealers,” Phys. Rev. Applied 8, 064025 (2017).

[12] A. D. King, J. Carrasquilla, J. Raymond, I. Ozfidan, E. Andriyash, A. Berkley, M. Reis, T. Lanting, R. Harris, F. Altomare, K. Boothby, P. I. Bunyk, C. Endreud, A. Fréchette, E. Hoskinson, N. Ladizinsky, T. Oh, G. Poulin-Lamarre, C. Rich, Y. Sato, A. Y. Smirnov, L. J. Swenson, M. H. Volkmann, J. Whittaker, J. Yao, E. Ladizinsky, M. W. Johnson, J. Hilton, and M. H. Amin, “Observation of topological phenomena in a programmable lattice of 1,800 qubits,” Nature 560, 456 (2018).

[13] M. Ohkawa, H. Nishimori, and D. A. Lidar, “Reverse annealing for the fully connected p-spin model,” Phys. Rev. A 98, 022314 (2018).

[14] D. Ottaviani and A. Amendola, “Low Rank Non-Negative Matrix Factorization with D-Wave 2000Q,” arXiv:1808.08721 (2018).

[15] D. Venturelli and A. Kondratyev, “Reverse Quantum Annealing Approach to Portfolio Optimization Problems,” unpublished (ACQ18) (2018).

[16] D-Wave Technical Whitepaper, Reverse Quantum Annealing for Local Refinement of Solutions (2018), https://www.dwavesys.com/sites/default/files/14-1018A-A_Reverse_Quantum_Aannealing_for_Local_Refinement_of_Solutions.pdf.

[17] T. Lanting, A. D. King, B. Evert, and E. Hoskinson, “Experimental demonstration of perturbative anticrossing mitigation using nonuniform driver Hamiltonians,” Phys. Rev. A 96, 042322 (2017).

[18] J. I. Adame and P. L. McMahon, “Inhomogeneous driving in quantum annealers can result in orders-of-magnitude improvements in performance,” arXiv:1806.11091 (2018).

[19] T. Albash, S. Boixo, D. A. Lidar, and P. Zanardi, “Quantum adiabatic Markovian master equations,” New J. of Phys. 14, 123016 (2012).

[20] V. N. Smelyanskiy, D. Venturelli, A. Perdomo-Ortiz, S. Knysz, and M. I. Dykman, “Quantum annealing via environment-mediated quantum diffusion,” Phys. Rev. Lett. 118, 066802 (2017).

[21] S. Boixo, V. N. Smelyanskiy, A. Shabani, S.V. Isakov, M. Dykman, V. S. Denchev, M. H. Amin, A. Y. Smirnov, M. Mohseni, and H. Neven, “Computational multiqubit tunnelling in programmable quantum annealers,” Nat. Commun. 7, 10327 (2016).

[22] A. J. Leggett, S. Chakravarty, A. T. Dorsey, Matthew P. A. Fisher, Anupam Garg, and W. Zwerger, “Dynamics of the dissipative two-state system,” Rev. Mod. Phys. 59, 1 (1987).

[23] R. Hanson, V. V. Dobrovitski, A. E. Feiguin, O. Gywat, and D. D. Awschalom, “Coherent Dynamics of a Single Spin Interacting with an Adjustable Spin Bath,” Science 320, 352 (2008).

[24] The transition time $t_r$ shown in Fig. 4 is calculated using the spectrum for a 12 qubit problem instance $T_{12}$ (spectrum shown in Fig. 22 of Appendix D). In this example, we do not calculate the full transition rates, but just use $t_r(s) \propto 1 - \exp(-\beta \omega(s))$ for demonstrative purposes. Here $\omega(s) = E_1(s) - E_0(s)$ and $\beta = 1/k_BT$ with $T = 12.1$mK. The other time scales shown $t_{\mu, p}$ are arbitrarily chosen.

[25] I. Hen, J. Job, T. Albash, T. F. Rønnow, M. Troyer, and D. A. Lidar, “Probing for quantum speedup in spin-glass problems with planted solutions,” Phys. Rev. A 92, 042325 (2015).

[26] Throughout this work the optimal pause point $s^opt$ is evaluated by finding the lowest average energy (from many thousands of anneals) returned from the D-Wave device. In principle one could use the ground state success probability as a metric, however this is often not practical since 1) some hard problems are not solved even once by the D-Wave, and 2) for randomly generated instances (i.e., not of the planted-solution type), the ground state energy is typically unknown.

[27] For a given problem, the later one can thermalize, the greater the ground state success probability, assuming the gap $\omega_0$ opens up so that e.g. the ratio $P_1/P_0 \propto \exp(-\beta \omega_0)$ is reduced.

[28] N. G. Dickson, M. W. Johnson, M. H. Amin, R. Harris, F. Altomare, A. J. Berkley, P. Bunyk, J. Cai, E. M. Chapple, P. Chavez, F. Ciotoa, T. Cirip, P. deBuen, M. Drew-Brook, C. Endreud, S. Gildert, F. Hamze, J. P. Hilton, E. Hoskinson, K. Karimi, E. Ladizinsky, N. Ladizinsky, T. Lanting, T. Mahon, R. Neufeld, T. Oh, I. Perminov, C. Petroff, A. Przybysz, C. Rich, P. Spear, A. Tcaciuc, M. C. Thom, E. Tolkacheva, S. Uchaikin, J. Wang, A. B. Wilson, Z. Merali, and G. Rose, “Thermally assisted quantum annealing of a 16-qubit problem,” Nat. Commun. 4, 1903 (2013).

[29] S. Aaronson and A. Arkhipov, “The Computational Complexity of Linear Optics,” in Proceedings of the Forty-third Annual ACM Symposium on Theory of Computing, STOC ’11 (ACM, New York, NY, USA, 2011) pp. 333–342.

[30] M. J. Bremner, R. Jozsa, and D. J. Shepherd, “Classical simulation of commuting quantum computations implies
collapse of the polynomial hierarchy," Proceedings of the Royal Society A: Mathematical, Physical and Engineering Science 467, 459 (2011).

[31] F. G. S. L. Brandao and K. Svore, “Quantum Speed-ups for Semidefinite Programming,” arXiv:1609.05537 (2010).

[32] T. Albash, V. Martin-Mayor, and I. Hen, “Analog Errors in Ising Machines,” arXiv:1806.03744 (2018).

[33] F. Wang and D. P. Landau, “Efficient, Multiple-Range Random Walk Algorithm to Calculate the Density of States,” Phys. Rev. Lett. 86, 2050 (2001).

[34] F. Wang and D. P. Landau, “Determining the density of states for classical statistical models: A random walk algorithm to produce a flat histogram,” Phys. Rev. E 64, 056101 (2001).
Appendix A: Expected closed-system dynamics

We consider the effect of an intermediate pause under the closed system (Schrödinger) evolution alone, studying 12-qubit problems, with $J_{ij} \in [-1, 1]$ (uniformly random) and $h_i = 0$.

It is interesting to note that the effect of pausing the anneal does have a noticeable effect, as demonstrated in Fig. 21, even in the closed system case. We believe this is essentially caused by Rabi oscillations during the pause, and we note it does not match the observed output from the D-Wave quantum annealer. We explain below.

We consider the three regions in Fig. 21 (bottom). 1) During the evolution, when $s < 0.2$ the state is almost entirely in the instantaneous ground state, $|\psi(s)\rangle \approx |E_0(s)\rangle$. Thus, when the system is paused, and evolved under $H(s_p)$, very little happens since just an overall global phase is acquired. 2) A little later on, when the energy gap starts to close between $s \in [0.2, 0.4]$ (see Fig. 22), diabatic transitions to excited energy levels may occur. Once a non-negligible amount of the population has been transferred to excited states, a pause will give rise to Rabi oscillations between the eigen-states of $H_p$, hence directly affecting the success probability at the end of the anneal. 3) Late in the anneal, after around $s = 0.7$, the driver Hamiltonian is essentially negligible, so can not drive any transitions between energy levels, hence a pause, will only change the relative phases of eigen-states of $H_p$, but not affect the probabilities upon measurement in the computational basis.

We describe three fundamental differences between the simulation, and the results from the experimental annealer (in addition to the large difference in success probability). Firstly it is evident there is much less structure in the closed system case; although the success probability $P_0$ against the pause point, for two different pause lengths ($t_p = 10, 1000\mu s$) as shown by the legend. The annealer data is from 10000 annealing runs, using 5 different gauges. Each plot contains 1000 data points evenly distributed in $s_p \in [0, 1]$. Both have an annealing time of $t_a = 1\mu s$ (in addition to the pause time). The simulation uses 1000 time steps in the calculation of the evolution operator.

It is interesting to note that the effect of pausing the anneal does have a noticeable effect, as demonstrated in Fig. 21, even in the closed system case. We believe this is essentially caused by Rabi oscillations during the pause, and we note it does not match the observed output from the D-Wave quantum annealer. We explain below.

We consider the three regions in Fig. 21 (bottom). 1) During the evolution, when $s < 0.2$ the state is almost entirely in the instantaneous ground state, $|\psi(s)\rangle \approx |E_0(s)\rangle$. Thus, when the system is paused, and evolved under $H(s_p)$, very little happens since just an overall global phase is acquired. 2) A little later on, when the energy gap starts to close between $s \in [0.2, 0.4]$ (see Fig. 22), diabatic transitions to excited energy levels may occur. Once a non-negligible amount of the population has been transferred to excited states, a pause will give rise to Rabi oscillations between the eigen-states of $H_p$, hence directly affecting the success probability at the end of the anneal. 3) Late in the anneal, after around $s = 0.7$, the driver Hamiltonian is essentially negligible, so can not drive any transitions between energy levels, hence a pause, will only change the relative phases of eigen-states of $H_p$, but not affect the probabilities upon measurement in the computational basis.

We describe three fundamental differences between the simulation, and the results from the experimental annealer (in addition to the large difference in success probability). Firstly it is evident there is much less structure in the closed system case: although the success probability does seem to increase on average, there is much more variability. This is due to the sensitivity of the period of the Rabi oscillations to the energy gaps (and hence to the location of the pause $s_p$). Second, there is seemingly no qualitative difference between a short and long pause in the closed system case, as compared to the observed phenomena which has the peak increasing with pause length. We believe this is due again to the nature of the Rabi oscillations. If the gap between energy levels is of the order of 1 GHz (see Fig. 22), the time-scale of the Rabi oscillations is much shorter than the pause lengths considered here (e.g. 1ns compared with 100µs). Lastly, the location at which this Rabi dynamics occurs does not correspond precisely to that observed in the experiment (it is seemingly shifted slightly earlier in the schedule).

We also plot both data sets on the same axis in Fig. 23 for reference. This shows the Rabi induced oscillations are effectively negligible compared to the effect observed.
on the physical annealer.

Appendix B: Computing the quantum Boltzmann distribution

We wish to compare the distribution returned from the D-Wave annealer, i.e., the probability that a configuration with energy \( E \) is returned \( P_{\text{DW}}(E) \), to what would be expected if the annealers were instantaneously thermalizing to the quantum Boltzmann distribution \( \rho(s,T) := \frac{1}{Z} e^{-\beta H(s)} \), where \( Z = \text{Tr} e^{-\beta H(s)} \), and \( \beta = 1/k_B T \) with \( T \) a temperature parameter.

We note that the D-Wave annealer can only measure in the computational \( (z) \) basis, and assuming the system can be quenched appropriately, to compare the probability distributions we compute

\[
P^{(s,T)}_{\text{QBM}}(E) = \sum_{z : H_p(z) = E} \langle z | \rho(s,T) | z \rangle \tag{B1}
\]

for \( s \in [0,1] \) (steps of 0.01), and \( T \in \left[ \frac{1}{4}, 4 \right] T_{\text{DW}} \) (steps of \( \frac{1}{4} T_{\text{DW}} \)).

Appendix C: Computing the classical Boltzmann distribution for large problems

In Sect. II E we analysed planted-solution type problems [25], of four different problem sizes, \( N \in \{31, 125, 282, 501\} \). These were (a subset of) the same instances as studied in Ref. [11], and are generated on subgraphs of the full chimera of side-length \( \text{SL} \in \{2, 4, 6, 8\} \) respectively. Each \( N \) group tested consisted of (at least) 55 problem instances, with a random number of sub-Hamiltonian loops chosen (as described in more detail in Ref. [11]).

The benefit to using this problem type is that one knows in advance the general form of the spectrum of \( H_p \), and one can calculate exactly the degeneracy of the ground and first excited states. The description of this algorithm is outlined in Ref. [8].

Knowledge of the exact ground and first excited state degeneracies is extremely powerful as it allows one to verify any estimated degeneracy values from entropic sampling techniques (such as the well known Wang-Landau method [33, 34]).

We used a newly devised algorithm for estimating the density of states based on population-annealing [10] to obtain accurate estimates of the degeneracies for the largest instances tested (501 qubits), for which traditional (e.g. Wang-Landau) approaches failed. Here ‘accurate’ implies neither the ground nor first excited state degeneracy estimate differed by more than 5% of the exact values. For the 125 and 282 qubit problems we were able to use the Wang-Landau algorithm to obtain accurate estimates of the degeneracies. For the 31 qubit instances we used exact enumeration to compute the degeneracies.

Appendix D: Supplemental figures

In Fig. 24 we show the full (working) D-Wave 2000Q hardware graph. All of our experiments were conducted on this graph.
FIG. 25. Success probability $P_0$ (under the default annealing schedule with $t_a = 1\mu s$) as a function of minimum gap $\Delta_{\text{min}}$ for the 100 problem instances of size 12 qubits reported on in the main text. We also plot the operating temperature of the annealer (black-dash line). The units are defined with $\hbar = 1$. The data is from 10000 anneals with 10 choices of gauge.

In Sect. II C we analysed 100 problems of size 12 qubits for which $J_{ij} \in [-1, 1]$ (uniformly random), and $h_i = 0$. In Fig. 25 we show how the success probability of these problems depends on the minimum gap $\Delta_{\text{min}}$. For problems for which $\Delta_{\text{min}}$ is larger than around 1GHz, the problems are solved with nearly 100% success probability.

In the main text (Sect. II A), one effect we studied was varying the total anneal time $t_a$, but keeping the pause length $t_p$ constant (e.g. Fig. 8). Here, in Fig. 26 we show the corresponding heat map (i.e. where $t_p$ is also varied for each choice of $t_a$). One sees that the pause is essentially an efficient way of increasing the success probability (lowering average energy) without increasing the anneal time; notice for a short anneal time, $t_a = 1\mu s$, with a pause of around 20$\mu s$ at $s \approx 0.4$ gives approximately the same average energy as an anneal for time of 1ms.

In Fig. 27 we show the spectrum of one of the 12-qubit problems from Fig. 13 which we classed as an ‘outlier’, due to it not having a well defined optimal pause point. We see the spectrum is quite different from one which has a well defined optimal pause point, e.g. Fig. 22, since the minimum gap occurs very late in the anneal, and does not open up much by the end of the anneal. It is interesting to note that all of the larger (> 100 qubits) problems tested had well defined optimal pause points, and therefore this is likely a small size effect.

Another interesting observation in Sect. II C was that by dividing the energy scale of the problem Hamiltonian, $H_p \rightarrow H_p/C$ for (e.g.) $C = 1, 2, 4, 8$, was that the peak in the success probability shifts to later in the anneal. This was partly due to the minimum gap which shifts to later in the anneal (see Fig. 28), but we also related this in the main text to the diminishing quantum fluctuations $Q$. In Fig. 29 we show the corresponding heat map for a single

FIG. 26. Effect of changing the total annealing time (not including the pause time), $t_a$, for a 501 qubit planted problem instance ($I_{501}$). The heat map color corresponds to the average energy, $\langle E \rangle - E_0$ (arbitrary units) returned from the annealer. From top to bottom the total anneal time $t_a = 1, 10, 100, 1000\mu s$ (see legend). In the bottom figure, with longest anneal time, the pause has little to no effect. Each data point is averaged from 5000 anneals with 5 different choice of gauge.
FIG. 27. (Top) Spectrum of one of the ‘outliers’ $T_{12}^{10}$ discussed in Sect. IID, which has a minimum gap late in the anneal ($s_{\text{gap}} = 0.77$), as shown in the figure. Also notice that the first excited energy level remains very close the the ground state all the way until $s = 1$. Note, the blue line which approaches $E_0$ around $s = 0.4$ is a ground state of $H_p$ (doubly degenerate ground state). (Bottom) Corresponding plot for the same instance where a pause of length $t_p = 1000\mu s$ is inserted into the anneal at point $s_p$. We see there is no clear peak (i.e. no optimal pause point), and in fact if one pauses around the location of the minimum gap there is a reduction in success probability, most likely due to excitations which do not have time to relax back down due to the gap occurring so late in the anneal. 10000 anneals, 10 gauges.

FIG. 28. Changing of the spectral properties upon re-scaling the problem. This is the same 12-qubit problem studied in Fig. 29 ($T_{12}^{12}$). The location of the minimum gap changes as $s_{\text{gap}} = [0.438, 0.508, 0.558, 0.608]$, and the minimum gap itself changes accordingly as $\Delta_{\text{min}} = [0.15, 0.10, 0.06, 0.03]$ GHz, when the problem Hamiltonian is re-scaled by $[1, 2, 4, 8]$ respectively (see legend). Energy units defined via $\hbar = 1$. Problem instance upon dividing the problem energy scale.
FIG. 29. Success probability $P_0$ heat map for a single 12-qubit instance ($I_{12}$) where the annealing schedule has a pause of length $t_p$ inserted at $s_p$, where from top to bottom the problem Hamiltonian $H_p$ has been re-scaled by a factor of 1, 2, 4, 8 (that is, $H_p \rightarrow H_p/C$, where $C = 1, 2, 4, 8$). See Fig. 28 for the corresponding minimum gap plot. Each data point is an average from 10000 anneals with 5 gauges. Notice the change in the color bar scale between the different images.