Quantum annealing has great promise in leveraging quantum mechanics to solve combinatorial optimisation problems. However, to realize this promise to its fullest extent we must appropriately leverage the underlying physics. In this spirit, I examine how the well known tendency of quantum annealers to seek solutions where higher levels of quantum fluctuations are present can be used to trade off optimality of the solution to a synthetic problem for the ability to have a more flexible solution, where some variables can be changed at little or no cost. I demonstrate this tradeoff experimentally using the reverse annealing feature a D-Wave Systems QPU for both problems composed of all binary variables, and those containing some higher-than-binary discrete variables. I further demonstrate how local controls on the qubits can be used to control the levels of fluctuations and guide the search. I discuss places where leveraging this tradeoff could be practically important, namely in hybrid algorithms where some penalties cannot be directly implemented on the annealer and provide some proof-of-concept evidence of how these algorithms could work.

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Introduction and background

Quantum annealing, in which combinatorial optimisation problems are mapped directly Hamiltonians and solved using sweeps of quantum parameters, has been a subject of much interest recently. This is in part due to the wide variety of potential applications, in a diverse range of subjects, including for instance air traffic control [1], hydrology [2], protein folding [3], flight gate assignment [4], finance [5, 7], and even quantum field theory [8]. This subject has further attracted interest because of the experimental maturity of the flux qubit devices produced by D-Wave Systems Inc. which allow for large scale experimentation.

One crucial direction in the growth of flux qubit quantum annealing is an increase in the variety of controls which users can be applied to the experimental quantum annealing process on flux qubit annealers. Traditionally formulated quantum annealing starts from an easy to prepare ground state of a so called driver Hamiltonian and monotonically interpolates the Hamiltonian to a problem Hamiltonian with an unknown ground state. However, major advantages can be gained by using a different control pattern known as reverse annealing, which starts in a state which is a guess for the solution of the optimisation problem, turns on fluctuations, and searches nearby states in Hamming distance by taking advantage of thermal dissipation [9]. Likewise, controls have been added which allow different qubits to be annealed differently [10].

These new features have proven useful in a variety of ways, reverse annealing for instance is motivated by the ability to implement more complex algorithms than traditional forward annealing [11], and these algorithms have shown promising initial experimental results. For example it was shown in [6] that starting from the output of a simple classical algorithm can lead to a large improvement over forward annealing. References [12, 13] showed that iterative methods can help over non-negative matrix factorization. The work in [14] showed experimentally that adding mutation performed using reverse annealing can aid the performance of genetic algorithms. Furthermore the simulation of the celebrated Kosterlitz-Thouless phase transition in [15] would not have been possible without reverse annealing techniques. Similarly, anneal offsets have shown promise in synchronizing the freezing of qubits [10].
The tendency of fluctuations to lead to uneven sampling of ground state manifolds has traditionally been viewed as a drawback for quantum annealing \cite{16, 17}. However, it has been observed that when coupled with classical techniques, this uneven sampling could be a positive feature because the states which quantum annealers find tend to be very different from those found by classical solvers, and therefore could give a more complete picture of the manifold \cite{18} if both were used together. In this paper, I explore a different advantage of this preferential search, the fact that it tends to find states which are flexible in the sense that some variables can be changed at little to no energy cost.

In this paper I experimentally investigate the role which quantum fluctuations can play in the local search which reverse annealing implements. This is done by using specialized Hamiltonians which represent hard problems for the annealer (although not necessarily hard in the computational sense) and have sets of local minima in their energy landscape where fluctuations are enhanced. I also show that the anneal offsets can be used to guide the search by locally enhancing fluctuations on some parts of the system. The technique of locally enhancing fluctuations is reminiscent of the methods proposed in \cite{20}, and provides some experimental validation of these concepts.

I use these fluctuations to trade of optimality in solutions for flexibility, in other words find solutions which are a bit less optimal, but for which certain variables can be changed at little or no cost. I argue that this is a property which is likely to be relevant in some real world situations and give a motivational example of how it can be used in a hybrid quantum classical algorithm to find a more optimal solution in the presence of a global penalty function which is not encoded into the annealer.

On the devices studied here (D-Wave 2000Q quantum processing units, QPU), dissipation plays an important (often positive \cite{21}) role in the annealing process, and the reverse annealing techniques used here fundamentally rely on dissipation. The intuition developed here however is likely to carry over into the more coherent protocols proposed in \cite{22, 23}. This is relevant because coherence rates can be improved through a variety of routes, both in superconducting flux qubit architectures \cite{25, 26}, and trapped ion quantum annealers \cite{27}. Furthermore, there is significant evidence that in the fully coherent regime fast quenches but coherent quenches, known as ‘diabatic’ quantum computing may be a promising path to a quantum advantage \cite{28}. This is due both to adiabatic mechanisms involving multiple energy levels \cite{29, 30}, and mechanisms related to energy transfer \cite{31, 32}.

This paper is structured as follows, first in section \ref{sec:setup} I describe the details of the experiment and discuss how the Hamiltonians used for the experiment are constructed. In section \ref{sec:exp} I give the core experimental results, demonstrating how fluctuations can enable a tradeoff between optimality and flexibility of solutions, as well as how anneal offsets can be used to guide the search by emulating these non-engineered fluctuations. Next in section \ref{sec:disc} I give a motivational example of how trading off optimality and flexibility can be useful. I then discuss some of the more detailed aspects of the experimental methods and concluded the paper with some discussion.

\section{Experimental Setup}

These experiments involve both specially engineered Hamiltonians to construct a search space with the necessary properties, and the use of advanced control features of the QPU, both anneal offsets and reverse annealing, which are used in combination. I first describe how the Hamiltonians are constructed, and than how they are used in the actual experimental protocols. Before, I do this, it is useful to provide some background on the operation of the quantum annealer. This QPU realizes a transverse field Ising Hamiltonian

\begin{equation} H = -A(s) \sum_i X_i + B(s) H_{\text{prob}}, \end{equation}

where $A(s)$ and $B(s)$ are non-linear functions of a control parameter $0 \leq s \leq 1$, $X_i$ is a Pauli $X$ acting on qubit $i$, and $H_{\text{prob}}$ is a programmable Ising problem Hamiltonian,

\begin{equation} H_{\text{prob}} = \sum_{ij} J_{ij} Z_i Z_j + \sum_i h_i Z_i, \end{equation}

where $Z_i$ is a Pauli $Z$ acting on qubit $i$, the details of how $J_{ij}$ and $h_i$ are chosen is discussed later.

The QPU is designed so that $A(0) \gg 1$ and $A(1) \ll 1$ and the ratio $A(s) / A(1)$ decrease monotonically with $s$. While the details of how these quantities depend on the annealing parameter $s$ is known, they are not important for this study beyond these basic facts. I do employ a more advanced feature known as anneal offsets, which slightly changes the form of Eq. (1) and will be discussed in due course.

\subsection{Hamiltonian Construction}

The goal of the experiments in this paper are to study the ability of a quantum annealer to use fluctuations to find high quality solutions which are flexible in the sense that changing some elements of the solution will not effect the energy of the solution, or will only affect it very little. Since I am not developing this study as a benchmark against classical methods, I have focused on designing Hamiltonians which are difficult to solve for the annealer, and have a known solution, but which are not necessarily computationally hard problems. To this end, the problems used here build on the planted solution construction from \cite{33}, which yields limited computational hardness \cite{34, 35} (for state-of-the-art solution planting techniques, see \cite{36}). Furthermore, I use many more clauses than
would be desirable to construct the hardest problems in the interest of ensuring that the problem graph is connected and to reduce the degeneracy of the ground state manifold.

The methods which I use, proposed in [33], constructs problems with planted solutions by generating overlapped frustrated loops on the edges of the underlying graph via random walks which terminate when they intersect their own path. I use planted solution problems with loop size greater than eight and 8,000 loops on a QPU with approximately 2,000 qubits (some of which are reserved for specialized features as discussed later in this section), with a coupling arrangement known as a chimera graph. Figs. [2] and [3] depict chimera graphs with a 3x3 grid of eight qubit unit cells, the 2000Q has the same eight qubit unit cells arranged in a 16x16 grid.

In addition to having a known planted solution, the experimental Hamiltonians also need features which can explore the ability of the annealer to use fluctuations to find more flexible solutions. Since I intend to study the ability to find more flexible solutions in both a binary and discrete setting, two different strategies need to be employed, gadgets where variables are allowed to become “free” should be embedded, henceforth referred to as “gadgets” as well as chains of qubits which encode discrete variables using the domain wall encoding described in [37], henceforth referred to as “chains”.

Fortunately, the planted solution construction does not require a full chimera graph to be effective. This means that the construction can be performed with some qubits reserved for either gadgets or chains, and these features can be added in later. The gadgets are constructed with the following properties:

1. Couplings to neighbouring qubits within the planted solution construction
2. A unique ground state when all external qubits which the gadget couples to are in the $|0\rangle$ (or $|1\rangle$) configuration
3. Degenerate ground state with free variables in cases where the external couplings do not agree, and therefore the planted solution components may be frustrated, these have equal energy to the unique state
4. Occupy a single chimera unit cell

Fig. [1] depicts a gadget which obeys these properties embedded into a larger problem Hamiltonian. The top row of Fig. [2] depicts the lowest energy states of this gadget when external qubits either agree or disagree. To be able to separate the effects of fluctuations due to free spins from other effects, I have also developed a ‘locked’ version of the free variable gadget, in this version some of the couplings are reduced to half the strength of the others so that the lowest energy state when the external variables do not agree no longer contains free variables, these are depicted on the bottom row of Fig. [2]

Figure 1: A free spin gadget inserted into a planted solution Hamiltonian. Green circles and dashed edges indicate qubits which are not part of the gadget, while black qubits indicate the active qubits within the gadget, with black edges indicating ferromagnetic couplers of unit strength and red edges indicating anti-ferromagnetic couplers of unit strength. Grey circles and edges indicate the unused couplers and qubits within the gadget. Pink colouring is used as a guide to the eye.

Figure 2: Top: Minimum energy state of free variable gadget with different configurations of external variables, left is where all external variables agree, right is where one disagrees. Bottom: Same but for locked gadget. Grey edges and circles indicate unused couplers and qubits, green indicates external qubits, red and black edges indicate anti-ferromagnetic and ferromagnetic coupling respectively, while thick edges indicates coupling of unit strength and thin indicate coupling with a strength of 0.5. Superimposed 1 and 0 characters indicate free variables. Slashes indicate frustrated couplings, with grey slashes indicating multiple possibilities depending on the values of the free variables.
For both the gadget and chain versions of the problem, ten Hamiltonians were created at random. Other than the reduced strength of the gadget couplings, the free and locked gadget runs use the same ten Hamiltonians. Each Hamiltonian includes either 15 gadgets or 15 chains.

B. Annealing protocol

The key feature of the Hamiltonians constructed for these experiments is that they have known planted solutions. This is crucial for the purpose of this study, to explore the ability of the device to trade off between optimality and flexibility, we need to start off in a state which is known to be optimal. Fortunately the reverse annealing feature [9] allows for a search around the planted (or any other classical) state. The reverse annealing feature uses a protocol which starts the QPU in a state determined by the user at $s = 1$, anneals to a value $s^*$ held for a time $\tau$ and then anneals back to $s = 1$ as depicted in Fig. [4]. Thermal dissipation allows the device to seek out lower energy states during the reverse annealing protocol.

In addition to the reverse annealing feature, I also make use of another feature called anneal offsets [10]. The function of this feature is to offset the annealing parameter on different qubits. In particular, I offset the parameter values of either the chains or the gadgets (a subset of qubits I call $g$), which makes the Hamiltonian

\[
H = -A(s) \sum_{i \in g} X_i + B(s) \left( \sum_{i \notin g, j \notin g} J_{ij} Z_i Z_j + \sum_{i \in g} h_i \right) - A(s + \delta s) \sum_{i \in g} X_i + B(s + \delta s) \left( \sum_{i \in g, j \notin g} J_{ij} Z_i Z_j + \sum_{i \in g} h_i \right),
\]

where $i \in g$ means that qubit $i$ belongs to a gadget or chain and $i \notin g$ means that it does not. The effect of these offset is to either locally enhance (negative $\delta s$) or suppress (positive $\delta s$) fluctuations locally within the gadgets or chains. The effect of combined anneal offsets and reverse annealing is depicted in Fig. [4].

For all experiments reported here, the anneals in the reverse annealing protocol were performed at the maximum allowed rate, which traverses from $s = 0$ to $s = 1$ in $5 \mu s$ and a hold time $\tau$ of $20 \mu s$ was used. The same parameters were used for chains and gadgets. For all values of $s^*$, I used a linearly spaced grid of 11 values of $\delta s$ evenly spaced between $-0.2$ to $0.2$, inclusive of the end points. Since not all qubits are capable of the full range of offset values, the maximum magnitude allowed (positive or negative) value was used when the desired value fell outside of the range. Because I wanted to study extreme values of $s^*$ as well as studying more values within a region of interest where the data were observed to change rapidly with $s^*$, I chose a the non-uniform grid of 19 values of $s^*$ depicted in Fig. [4].
In this section I discuss the results of the experiments, which demonstrate how both existing and introduced fluctuations can be used to guide the search which a quantum annealer performs. First I will introduce how the number of free gadgets or soft chains can be controlled by different parameters, such as the value of $s^{\star}$ and the anneal offsets applied to the chains or gadgets. Measures of the performance of these different control settings will be introduced in Sec. II.A and further discussed in Sec. II.B. A proof-of-principle example for how guided search can be useful will be discussed in Sec. III.

The first result which we find is that the number of free gadgets and soft chains both can be increased by decreasing the value of $s^{\star}$, in other words by increasing the range of the search. Fig. 6 shows this effect for gadgets, not only are more gadgets free the lower value of $s^{\star}$, this effect is also much stronger when the gadgets are not locked, indicating that the free variables have a significant effect on the dynamics. For $s^{\star} \gtrsim 0.45$ the dynamics are highly localized and very few if any gadgets are free, meanwhile for $s^{\star} \lesssim 0.38$, the behaviour is indistinguishable from a search with $s^{\star} = 0.2$, effectively a global search. I have chosen a non-uniform mesh of $s^{\star}$ values which focuses on the regime where the reverse anneal can lead to long range dynamics, but does not search so far that all information about the initial state is completely forgotten.

Fig. 7 shows the same effect for embedded chains in planted solution problems. In this case, reducing the fluctuations by increasing the hardness coefficient leads
to fewer soft chains. As with the gadget example, non-
trivial reverse annealing dynamics are seen for $0.38 \lesssim s^* \lesssim 0.45$.

We further observe that if we apply anneal offsets to
the locked gadgets, we can mimic the effect of the free
variables, as Fig. 8 shows the proper choice of anneal
offsets renders the distributions indistinguishable for the
locked and unlocked gadgets. I show in sec. IIB that
introduced fluctuations from anneal offsets can be as ef

tive if not more so than fluctuations due to truly free

The question now becomes whether anneal offsets can
similarly mimic the effect of a lower hardness coeffi
cient for chains within the planted solution Hamiltonian.

Fig. 9 indicates that it cannot, while a negative anneal
offset parameter, $\delta s < 0$ increases the number of soft
chains at intermediate values of $s^*$, it decreases the num
ber at low $s^*$. Therefore no value can be used to mimic
the behaviour of a lower hardness coefficient simultane-
ously in both regimes. This is likely due to the more com
plicated structure of the chain encoded discrete variables.
I demonstrate in sec. IIB that in contrast to the locked
versus unlocked gadget example, anneal offsets cannot
make up the difference between the minimum and maxi
mum hardness of the chains.

A. Conditional performance

Simply analysing solution optimality is a losing propo
sition, since I have designed the experiments such that,
by construction, there is no way of improving beyond
the starting condition. However, there is still hope to
find high quality solutions which meet conditions which
the global solution does not. I define this as conditional
performance, the best performance attainable which also
meets certain conditions. Because of how the gadgets
and domain wall variables have been constructed, the
condition I have chosen to analyse is how many gadgets
can be in the free configuration, or chains can be in a
soft configuration. This is an interesting criteria since
free gadgets and soft chains both make the solution more
flexible, allowing for modifications which can be made
with little or no energy cost. This flexibility could be
important in real world scenarios, for instance if small
changes to the solution may need to be made after the
time of solving to account for unpredictable events, or
if the annealer is being used as part of a hybrid solv
ing technique where difficult to encode global constraints
are not included (for an example of the latter see [6]). In
Sec. III I give an example where flexible solutions can be
used to gain an advantage when an additional non-linear
constraint is added.

For a fair comparison, we should compare the results
from the annealer with a trivial classical strategy of
simply frustrating the couplings between the gadgets or
chain and the rest of the problem, this ‘trivial’ strategy
leads to a cost per gadget or chain of 2 energy units
compared to the most optimal solution. Solutions with
a lower cost per gadget/chain, are in principle interesting
solutions, whereas those which have a higher energy
than the trivial approach are not, since there is a know
method which will always attain a better solution us
ing the same starting information. Since the focus of
this work is proof-of-concept rather than benchmarking,
I will not explore whether or not there are other, less
trivial, classical algorithms which can have better condi
tional performance than the annealer.

Figure 8: Fraction of observations for different numbers of
gadgets free against different values of $s^*$ averaged over all 10
Hamiltonians solid red lines with ‘X’ markers represent the
mean for the plot, while the dashed line with ‘+’ markers is
the mean of the other plot for comparison. Top: Unlocked
gadgets with no anneal offsets. Bottom: Locked gadgets with
anneal offsets ($\delta s$) of up to $-0.04$ applied to the gadgets. The
methods for creating the plots given the non-linear mesh are
explained in Sec. IV

Figure 9: Fraction of observations for different numbers of
chains soft against different values of $s^*$ averaged over all 10
Hamiltonians solid red lines with ‘X’ markers represent the
mean for the plot, while the dashed line with ‘+’ markers is
the mean of the other plot for comparison. Top: Chains with
maximum hardness coefficient and no anneal offsets. Bottom:
Chains with maximum hardness coefficient and offsets ($\delta s$) of
up to $-0.04$ applied to the gadgets. The methods for creating
the plots given the non-linear mesh are explained in Sec. IV
To start off, let us examine the conditional performance for the Hamiltonian with gadgets inserted without using anneal offsets. As Fig. 10 shows, even without anneal offsets the annealer is able to outperform a trivial algorithm in all but one case, in which the energy cost is more only if every gadget is made free. When different anneal offsets on the gadgets are allowed, the energy cost per free gadget never exceeds 1.5.

For discrete variables represented as domain walls, reverse annealing is also usually able to find a solution which beats the trivial approach, in fact Fig. 11 shows that even without using anneal offsets, the annealer was always able to find a solution which was better than the trivial approach when the soft region of the chain is flat (softness parameter $s$ of 0). Even when the region of the chain which is being searched out is not flat, but a sloping minima (softness parameter $s$ of 1), the annealer is able to beat the trivial approach in most cases, and always does both on average, and for all cases examined with less than 14 soft chains. The results for the higher softness parameter are depicted in Fig. 12.

I have now shown that reverse annealing in combination with anneal offsets can be effective at modifying solutions to meet certain conditions, but have not elucidated why or how this might happen, in the next subsection I examine potential underlying mechanisms and discuss what the data can teach us about anneal offset strategies.

### B. Performance with anneal offsets and locked gadgets

It is now worth examining more closely the role which quantum fluctuations play in conditional performance, by comparing Fig. 11 and 12 (averages directly compared in Fig. 13 (left)). We are able to see that better solutions are possible with a lower softness parameter $s$, the question we have not explicitly answered yet, is whether the same is true for the fluctuations the free spins cause in the gadgets. To do this we need to compare the ‘free’ and ‘locked’ versions of the gadgets as introduced in Sec. I. As Fig. 13 (right) shows, in the absence of anneal offsets having locked gadgets is very detrimental to performance, at least if more than about 6 gadgets are desired to be free. On the other hand there is barely any difference once anneal offsets are employed, suggesting that the offsets can enhance the fluctuations and guide the search. Conversely, the effect of anneal offsets seems to be rather minimal for discrete variables encoded in chains.

The first question to ask is what is the optimal value of $s^*$ for given a desired number of free gadgets and soft chains, and how is this affected by factors like whether or not gadgets are locked and the softness parameter used.
for gadgets, and does not change it as much for chains. Furthermore, except for when about 14 or more free gadgets are desired, the optimal value of $s^*$ when anneal offsets are used is almost the same for locked and unlocked gadgets, supporting the hypothesis that increased fluctuations from anneal offsets can act as an effective proxy for truly free variables.

To better understand the role anneal offsets are playing, it is worth examining how the best choice of anneal offset depends on the number of free gadgets, or soft chains desired. As Fig. 15 shows, the best strategy is indeed to use stronger offsets in the locked gadget case, and to use them to enhance rather than suppress fluctuations on the gadgets, suggesting that there is indeed a mechanism where offsets artificially guide the search by making the locked gadgets behave as if they have free qubits.

Fig. 15 further shows that domain wall encoded discrete variables show very different behaviour to the gadgets, in particular, up to statistical uncertainty, the offsets used in the discrete variable case monotonically approaches zero as more soft chains are desired, while for gadgets with free binary variables, there non-monotonic behaviour, and a trend toward locally enhancing fluctuations if more free gadgets are desired. This difference is likely due to the more complex structure of the domain wall encoded variables, leading to less tolerance to fluctuations before they no longer faithfully encode the intended variable.

III. MOTIVATIONAL EXAMPLE FOR FLEXIBLE SOLUTIONS

Now that we have shown that the underlying dynamics of quantum annealers can be used to find solutions which
are more flexible, it is worth demonstrating an example where such solutions could be useful. To do this, we consider a problem which natively fits onto the chimera graph, but is also subject to global non-linear penalty. Such global penalties are likely to be encountered in realistic problems, and for example may arise when a shared resource is being used for different purposes and there is a penalty which depends on the total amount required. A simple example of how such a constraint could arise in the real world is minimising the total cost of a project if a company owns \( X \) number of a piece of equipment, so there is no penalty for a solution which uses any number up to \( X \), however there is a cost associated with renting every additional piece of equipment beyond the original \( X \).

While techniques are known to implement global non-linear penalties on quantum annealers, for example those proposed in [38,39], these techniques require a fully connected graph and number of auxiliary qubits equal to the number of original qubits, such an encoding is not practical for large problems on existing quantum annealers. We consider an alternative strategy for solving such problems, we first encode the entire problem except for the global penalty onto the annealer, and use reverse annealing techniques to find solutions with various levels of trade-off between flexibility (for example measured by the number of free gadgets) and optimality. I then perform greedy optimisation as described in the methods section starting from the best solution found at each level of flexibility. This greedy optimisation is performed against the entire problem including the non-linear penalty.

Before considering the results for the QPU-sized problems used in earlier demonstrations, it is worth demonstrating this approach with a simpler 16 qubit example. To do this, we consider the Hamiltonian used in [21]. Similarly to the Hamiltonian considered in [40]. This Hamiltonian has both a local minimum where eight of the 16 qubits are “free”, able to exist in either the zero or one state without incurring an energy penalty, and a global minimum where none of the qubits are free, the (unique) ground state and first excited state manifold of this Hamiltonian are depicted in Fig. 16. At least for short runtimes, the close avoided crossings in these devices mean that quantum annealers will typically find the false minimum with more free qubits due to a close avoided crossing relatively late in the annealing schedule [21].

We now consider the ability of the solution to adjust to non-linear penalties of different strength. The global non-linear penalty I elect to use is non-linear function of the Hamming distance \( D \) from a random state

\[
E(D) = 1 - \exp\left(\frac{(D - \left(\frac{n}{2} + \sqrt{n + 1}\right))^2}{n + 1}\right),
\]

where \( n \) is the number of qubits involved in the Hamiltonian. The states which the annealer returns will be a Hamming distance \( D = \frac{n}{2} \) away from most random states, therefore this penalty offsets the Gaussian from the point where a typical solution will sit by its standard deviation, \( \sqrt{n + 1} \). This will guarantee that the non-linear penalty will have a substantial gradient for typical starting states.

Equipped with this definition we consider the results of adding a non-linear penalty followed by a greedy search for the 16 qubit problem mentioned earlier. As Fig. 17 shows, it is much easier for the greedy search heuristic to compensate for the global non-linear penalty starting from the higher energy but more flexible solution which the annealer finds as compared to the true minimum, the result is that for moderate penalty strength, the more flexible state is a superior choice for a starting configuration.

A. Synthetic use case: optimizing with global non-linear penalties

We now consider what happens when we apply a non-linear penalty followed by greedy search to states with different numbers of free gadgets found for QPU scale problems. While neither the original problem, nor the non-linear penalty are based on anything which one might encounter in the real world, recall that situations where a problem containing a non-linear penalty must be solved are realistic, this can therefore be considered a “synthetic” use case for a quantum annealer, not directly based on an application, but with a structure which is likely to be encountered in the real world. We start by considering the best solutions the annealer could find.
with different free gadget numbers for a single Hamiltonian, in this case Hamiltonian number 7. As Fig. 18 shows, as the penalty strength is increased to a moderate value, the best solution is no longer obtained from starting a greedy search at the true energy minimum, but from starting with a more flexible state with more gadgets free. For these experiments I only consider the best solution found with each number of gadgets free, choosing at random in the event of a tie.

From Fig. 19 we can see that the behaviour seen in Fig. 18 is indeed typical of results found both with and without anneal offsets although, unsurprisingly, the cases where anneal offsets are used perform better on average since lower energy solutions can be found by using anneal offsets.

Finally, we consider the optimal number of free gadgets in the starting state for different Hamiltonians and penalty strengths. Fig. 20 shows that, for both the strategy using anneal offsets, and the one which does not, the typical number of gadgets free in the best performing state increases for a while with penalty strength and then settles to an average across all Hamiltonians of around seven gadgets free. While it is possible that the average number of gadgets free is slightly higher for the strategy using offsets, the difference is relatively small. It is however clear that for the solutions which used anneal offsets, there is a much wider variety of solutions, and in particular, a tendency to use some solutions with many more gadgets free.

IV. METHODS

All reverse annealing experiments were performed using the maximum allowed annealing rate on both the forward and reverse anneal, at this rate the entire (forward) anneal would be completed in 5 $\mu$s. All experiments used a hold time $\tau$ of 20 $\mu$s. All annealer calls were set to perform 1,000 individual runs. The reverse annealing experiments presented here were performed using the D-Wave.
Matlab API between 27 October 2018 and 30 October 2018 on a commercially available D-Wave 2000Q QPU with QPU time purchased by BP plc. Data are publicly available at [41].

Greedy optimisation was performed by checking all single bit flips and performing the one which reduces the energy the most, choosing at random in the event of a tie. The greedy procedure is repeated until no single bit flip will reduce the energy.

All plots were produced in the Python language [42] and the matplotlib plotting package [43]. code used to produce the plots and perform the experiments is available from the same public repository as the experimental data. Heat-map plots with non-linear grids were plotted such that the centre of each cell aligns with the value of each axis. The NumPy [44] and SciPy [45] packages were also used as well as jupyter notebooks [46] and the IPython interpreter [47].

V. DISCUSSION AND CONCLUSIONS

In this paper, I have demonstrated how fluctuations can guide quantum annealers to trade off optimality for more flexible solutions, as well as motivated cases where such a tradeoff could be useful. The particular useful case I focus on is when a problem involved global penalties which cannot practically be implemented on the annealer. While in the past the tendency of quantum annealers to find solutions where fluctuations are stronger has been seen as a weakness, for instance in inhibiting the ability to uniformly sample ground states, I demonstrate ways in which it could be useful.

In addition to demonstrating that the existing fluctuations on the annealer can help guide searches toward more flexible states, I show that locally offsetting the annealing schedule of the qubits can be used to guide the search. This provides experimental motivation for methods like those proposed in [20], which incorporate bitwise uncertainty into algorithms.

While not explored here, it is likely that analogous effects could be seen in quantum inspired algorithms based on spin like systems, for example quantum Monte Carlo techniques [48] which should show analogous effects to the fluctuations observed here. In fact the proof-of-concept numerics in [20], exhibited that fluctuations can attract quantum Monte Carlo dynamics preferentially to some minima over others. This work has introduced new ways in which quantum annealers and related algorithms can be used, beyond directly finding the most optimal solution, an important direction in hybrid quantum-classical computing. By laying the groundwork for how modifying fluctuations locally can be used algorithmically to guide a search, the work here opens a new path to using these modified fluctuation strengths algorithmically, in a similar vein to currently used reverse annealing techniques, but guiding the direction of the search, rather than the starting point.

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Appendix: Review of the domain wall variable encoding strategy

The domain wall encoding strategy used here was originally developed to undertake the research described in this paper, since it can encode discrete variables on a chimera graph without requiring minor embedding unlike the more traditional one-hot strategy. Because the domain wall encoding strategy has been observed to significantly out perform the one-hot strategy on several key metrics related to embedding on realistic hardware graphs, a full description of this technique as well as numerical evidence of its superior performance has been published elsewhere [37], and an experimental study of its comparative performance to one-hot is forthcoming [19]. This technique has also been used in solving quantum field theory problems using quantum annealers [8].

In the interest of making the current paper self-contained, I review the basics of the domain wall encoding and some of it’s key features. As Fig. 21(top), shows, the domain wall encoding is produced by creating a linearly connected chain of $n - 1$ qubit with frustrating fields on each end such that there are $n$ total possible domain wall locations, including frustrating the the fields at either end, which can be thought of as couplings between the terminal qubits and “virtual” qubits which are
Evgeny Andriyash, Zhengbing Bian, Fabian Chudak, arbitrary penalties can be realized by putting fields (single
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between the qubits in the domain wall encoding, and ar-
bitary penalties can be realized by putting fields (single
body terms) on the chain. Moreover, the domain wall
encoding of a binary variable simply reduced to a normal qubit representa-
tion, as depicted in Fig. 21 (bottom).

I am interested in simple couplings which force frustra-
tion in the planted solution problem if the domain wall
variable takes one of its soft values, while simultaneously
avoiding the need for minor embedding. To do this, I
place a single ferromagnetic coupler between the qubits
encoding the discrete variables and the other qubits at
each end of the soft region. For the additional energy
penalties on the chain, I make use of the fact that a single (non-extreme) value of the discrete variable can be
penalized using a term of the form $\delta_i = \frac{1}{2}(Z_i - Z_{i-1})$. For the extreme values can be penalized in the same way, but
omitting terms which correspond to virtual qubits. This
method is described in more detail in [37], and software
for realizing these encodings can be found at [50].

Figure 21: Top: Encoding of a discrete variable as a domain
wall position, the domain wall is depicted in blue, real qubits
in green and `virtual` qubits which are fixed are depicted in
pink with dotted borders. Bottom: A binary variable in the
domain wall position, the domain wall is depicted in blue, real qubits
in green and _virtual_ qubits which are fixed are depicted in
pink with dotted borders.
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