Final Project Report
Quantum Annealing: An Overview

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1 Introduction

The prospect of leveraging quantum phenomena to perform complex, and often classically intractable, calculations has captured the imagination and interest of physics for a few decades. In the archetypal vision of quantum computing (circuit model), we apply a series of unitary-gate operations on a collection of two-state systems, or quantum bits (qubits). Importantly, entanglement between qubits allow uniquely quantum algorithms such as quantum teleportation, quantum speed-ups, and quantum error-correction [1].

In addition to the circuit model, many other paradigms for quantum computing have been developed. To name a few: topological quantum computing, measurement-based quantum computing, and adiabatic quantum computing [2]. This project focuses on quantum annealing, a technique in the family of adiabatic quantum computation.

As a prelude to the project, the primary shift in thinking between circuit-model and adiabatic quantum computation is that instead of manipulating qubits via a set of discrete gates, quantum annealing attempts to encode computation in the process of evolving a Hamiltonian to its ground state.

2 Simulated Annealing

To gain motivation and intuition for quantum annealing, we begin by discussing its classical analog and predecessor: simulated annealing.

Simulated annealing is a general technique for solving hard optimization problems [3]. Specifically, combinatorial optimization problem where we wish to optimize (i.e. without loss of generality, finding the minimum) a multivariate function with with a finite set of inputs for each variable. Furthermore, we're generally interested in problems without a known solution in polynomial time (NP).

2.1 Spin Glass

One such problem is finding the ground state of a spin glass. A spin glass can be represented by an Ising model with random ferromagnetic or antiferromagnetic interactions between lattice points. The spin of each site can be flipped in search of a lower energy state.

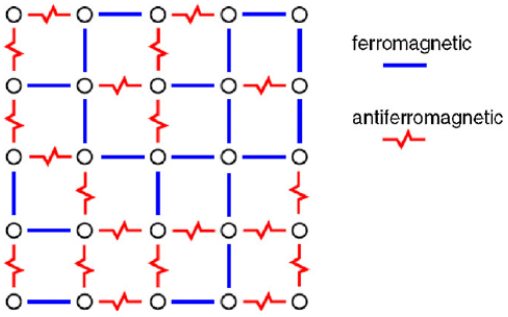

Figure 1: A two-dimension spin glass. Image source: [4]

The problem of finding the ground state is challenging because the system is frustrated: competing interaction between spins at each lattice site prevents all sites from evolving to its minimum energy. This means that there is no clear path for the system to lower its energy. For example, a series of spin flips might reduce the energy of the system in the short term, but lead the system down an unfavorable path in the long term. If we were to plot the energy of a spin glass system in configuration space (i.e. as a function of all possible configurations), we expect the landscape to be very rugged and with many false, local minimums.

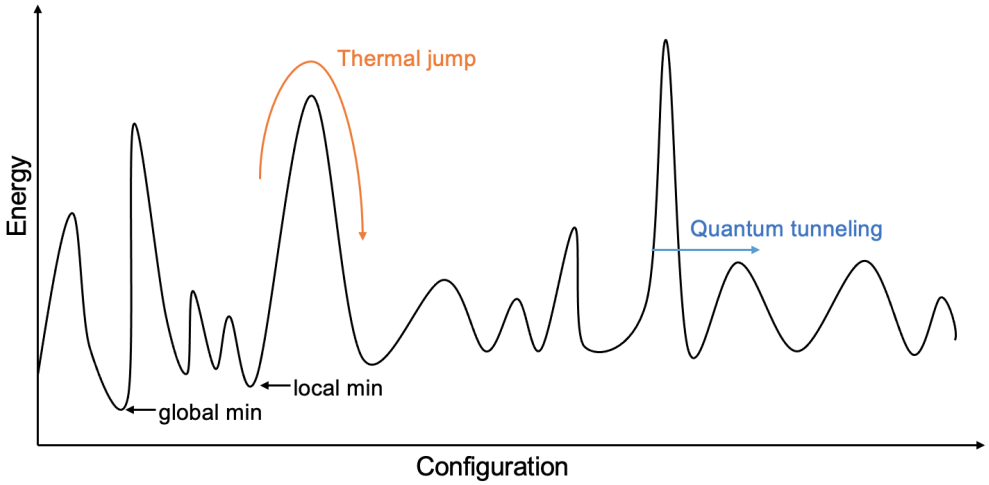

Figure 2: The energy landscape of a hard-to-solve optimization problem. Many local minimums are surrounded by high potential barriars. Thermal jumps and quantum tunneling can allow the system to escape false minimums. Inspiration: [3]

This "glassy" behavior is common to many optimization problems and is why they are challenging to solve via classical means. In the case of a spin glass with with N sites, we would need to examine 2^N possibilities in order to explore the entire configuration space.

A naive approach to solving this problem would be a greedy algorithm: starting the system in a random state, the spin glass is only allowed to move to lower energies until it has reached a minimum. While this is effective at finding *a minimum*, it is unlike to be the *global minimum* in such a rugged energy landscape.

Simulated annealing is a simple modification of this algorithm. While the system still has a general tendency to seek lower energy, in order to prevent it from settling too quickly into a local minimum, thermal fluctuations are introduced to periodically bump the algorithm past high energy barriers (figure 2) and away from false minimums. We shall defer a more detailed examination of simulated annealing for the following section.

2.2 Traveling Salesman Problem

We now turn to the traveling salesman problem (TSP) to show a simple implementation of simulated annealing and to explore some run-time properties.

The TSP states that: given a list of cities and the distances between each pair of cities, what is the shortest tour that visits each city exactly once and returns to the origin city?

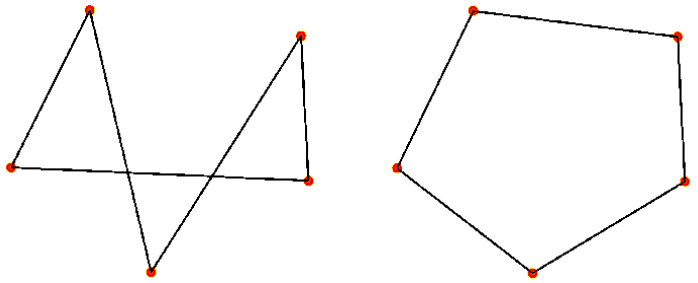

Figure 3: A 5-city problem with two unique tours. By simple examination, we see that the right tour is more optimal.

To provide a tangible example of simulated annealing, I created an interactive simulated annealer of the TSP available at https://www.ocf.berkeley.edu/~yizhu/sa.html.

Following the process detailed in the previous section, the simulation works as follows:

1. The TSP system starts at a random initial state and an initial temperature T_0. We define a heuristic for energy, which, in the case of the TSP, is the Euclidean tour length.
2. In order to generate permutations of the current state, we need a mapping that takes a valid tour to another valid tour. This simulation uses the 2-opt move: for two paths $A \to B$ and $C \to D$, after the swap, the paths becomes $A \to D$ and $C \to B$.
3. For each time step, the algorithm explores a new tour given by a random 2-opt move. If the system had an initial energy of E_i and a new energy of E_f, the probability of the system accepting the new tour is given by the Boltzmann factor,

$$P = \min\{1, \exp\left(-(E_f - E_i)/T\right)\} \tag{2.1}$$

4. The temperature of the system is reduced according to some annealing schedule and the previous step repeats until the temperature has reached zero.

From the procedure above, we see that the system will always evolve to a state of lower energy. However, if we encounter a higher energy state, there will be some probability of evolving to that state depending on both the energy difference (the unfavorability of the state) as well as the current temperature.

This random thermal fluctuation allows the algorithm to explore more of the configuration space and avoid being trapped at a local minimum. However, the system eventually converges on a minimum because we lower the temperature as time goes on so that the algorithm become more and more adverse to higher energy states. This slowly "anneals" the system to a close-to-optimal state.

As with metallurgic annealing, the rate of the annealing process has a large impact on the final result. We can imagine that if we cool the system very quickly, the algorithm will

not have an adequate chance to explore the configuration space and will converge to a sub-optimal result.

There have been several attempts are more rigorously quantifying the annealing rate. Commonly cited is the following theorem [5, 6]

Theorem 1: *suppose S^* is the optimal state and d^* is a measure of the difficulty for the system to escape from a local minimum to S^*. Then the simulated annealing algorithm converges if and only if,*

$$\lim_{t\to\infty} T(t) = 0 \tag{2.2}$$

and

$$\sum_{n=1}^{\infty} \exp[-d^*/T(t)] = \infty \tag{2.3}$$

where $T(t)$ is the annealing schedule.

One interpretation of this theorem is that if we have a local minimum of depth d^*, then the probability of escaping the well at some time is $\exp[-d^*/T(t)]$. Thus, the condition given by equation 2.3 is essentially that after an infinite number of trials, the algorithm is guaranteed to escape the local minimum because the sum of the probabilities is infinite [7].

This also seems to "naturally" suggest that we adopt the annealing schedule,

$$T(t) = \frac{d}{\log(t)} \tag{2.4}$$

for some constant d.

However, literature at the moment suggests that there are no convincing arguments that this annealing schedule 2.4 is superior to a constantly-decreasing-temperature schedule. Furthermore, there appears to be a lack of a rigorous constraint on the convergence rate [7].

Instead, we return to our implementation of TSP annealing.

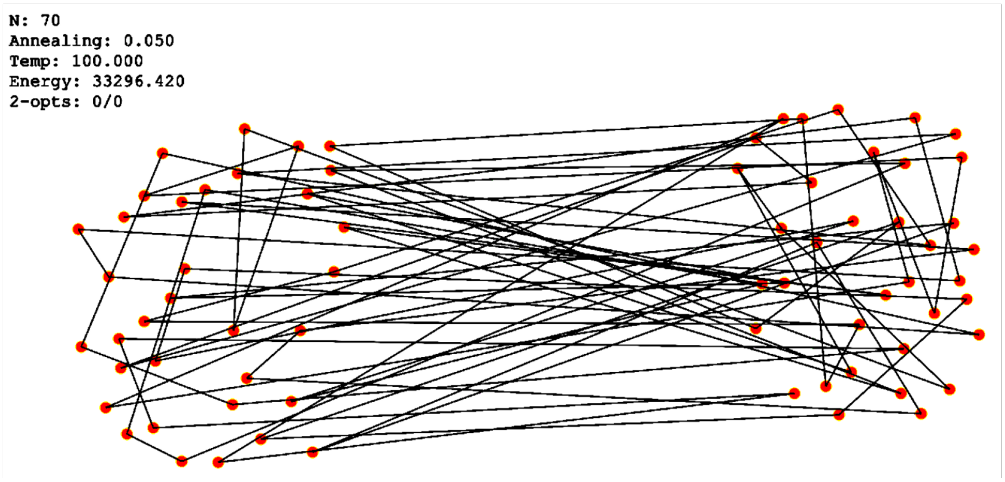

Figure 4: A highly inefficient starting state of a 70-city TSP.

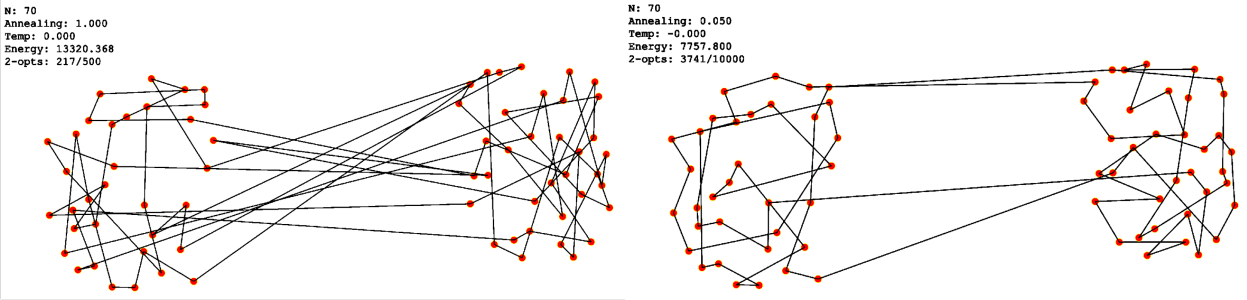

Figure 5: Final annealed states of the 70-city TSP. A linear annealing scheme with a starting temperature of 500 was implemented. (a) fast annealing: 1.00 degree per time step for a total of 500 $\sim O(N)$ steps. (b) slow annealing: 0.05 degree per time step for a total of 10000 $\sim O(N^2)$ steps.

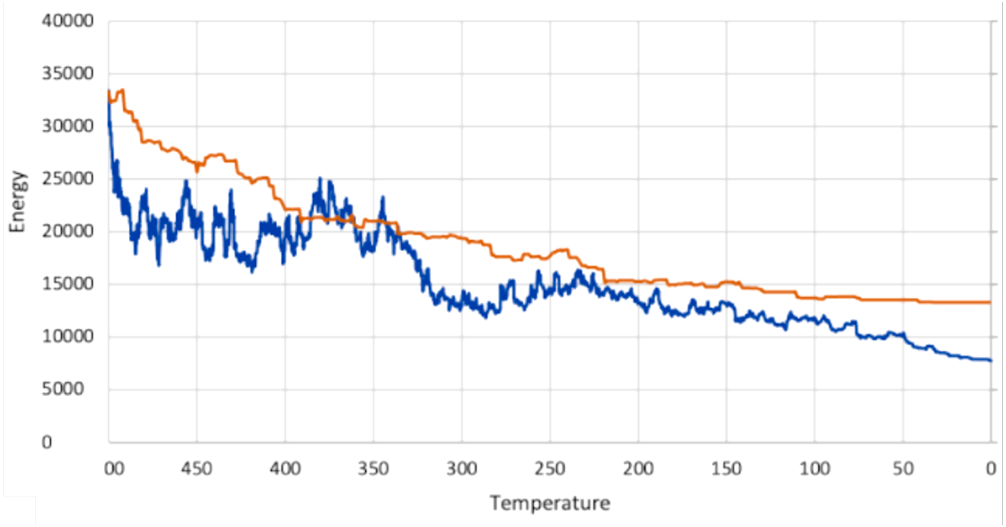

Figure 6: Energy as a function of time for the different annealing rates of the 70-TSP: fast annealing (orange) and slow annealing (blue). The faster annealing curve is much more smooth, an indication that less of the configuration space is explored. The jagged edges of the slower curve is an indication of the algorithm exploring then leaving various local minimum.

From figures 4, 5, and 6, we can see more qualitatively the impact of annealing rate. Furthermore, from figure 5, we can say—non-rigorously—that on the order of polynomial time, simulated annealing can yield fairly optimal results. Note that simulated annealing is a very effective general optimization technique, but there are faster TSP-specific algorithms [3].

3 Quantum Annealing

Quantum annealing is the quantum analog of simulated annealing. Abstractly, instead of thermal fluctuations driving the annealing algorithm, we introduce quantum tunneling as the primary means to escape false minimums (figure 2).

Utilizing quantum versus classical phenomena has two benefits. Firstly, quantum tunneling introduces classically unlikely paths through the configuration space despite potentially high energy barriers. In addition, in the early stages of annealing, the wave function of the qubits is delocalized over the entire configuration space, this is analogous to allowing the wave function to explore the entire space at once [3].

The process of optimizing a problem function using quantum annealing is as follows. First, we define a mapping between the problem and an Ising Hamiltonian,

$$\mathcal{H}_{\text{Ising}} = \sum_i h_i \hat{\sigma}_z^{(i)} + \sum_{i>j} J_{ij} \hat{\sigma}_z^{(i)} \hat{\sigma}_z^{(j)} \tag{3.1}$$

In other words, we must define our problem such that its inputs can be mapped to a collection spin states (with various interaction energies) and the lowest energy state of the system corresponds to the optimized solution.

Next, we set up a time-dependant Hamiltonian,

$$\mathcal{H} = A(t) \underbrace{\left(\sum_i h_i \hat{\sigma}_x^{(i)} \right)}_{\text{transverse-field term}} + B(t) \underbrace{\left(\sum_i h_i \hat{\sigma}_z^{(i)} + \sum_{i>j} J_{ij} \hat{\sigma}_z^{(i)} \hat{\sigma}_z^{(j)} \right)}_{\text{Ising term}} \tag{3.2}$$

Where h_i is an external field term and J_{ij} is the interaction term. Initially, the system starts in the ground state of the transverse field Hamiltonian. In other words, for $B(t=0) = 0$ in equation 3.2, the starting state is an even superposition over the computational basis.

As time evolves, we anneal by slowly increasing the influence of the Ising term while reducing the influence of the transverse field term. At the end of the annealing process at time t_f, $A(t = t_f) = 0$ and only the Ising term remains.

If this annealing process occurs at sufficiently slow rate, we expect that the system will remain in the ground state of the Hamiltonian throughout all time. Thus, at the end of the quantum anneal, we expect our qubits to be in the ground state of our problem Ising Hamiltonian and we have arrive at our solution!

Similar to the convergence theorem (Theorem 1) for simulated annealing, the Adiabatic theorem provides a more rigorous lower bound on the time complexity of quantum annealing. A coarse description of the Adiabatic theorem stipulates that the condition for the wave function of the qubits to remain in the ground state is the *approximate* inequality [8],

$$\max_{t \in [0, t_f]} \frac{|\langle \varepsilon_1(t)| \, \partial_t \mathcal{H} \, |\varepsilon_0(t)\rangle|}{|\varepsilon_1(t) - \varepsilon_0(t)|^2} \ll t_f \tag{3.3}$$

Where ε_i is the energy of the ith energy eigenstate. If we define,

$$\Delta = \min_{t \in [0, t_f]} \varepsilon_1(t) - \varepsilon_0(t) \tag{3.4}$$

then equation 3.3 suggests that that the annealing time should be on the order of $O(1/\Delta^2)$ [9]. In other words, we expect the run time to scale as the inverse square of the minimum energy gap between the ground and first excited state.

3.1 TSP with Quantum Annealing

In the previous section, we showed an implementation of TSP with simulated annealing. Similarly, we can approach the traveling salesman problem with quantum annealing. For the sake of brevity, we shall skip the details of the implementation and simply emphasize the most important points: the TSP can be mapped can onto an Ising Hamiltonian. In addition—and very importantly—it is possible to further constrain the system so its evolution from a starting state of a valid tour will remain a valid tour (e.g. evolution via the 2-opt move described previously). Thus, annealing the TSP-Hamiltonian is equivalent to finding an optimal solution.

Using a path-integral Monte Carlo method to simulate the dynamics of quantum annealing, a study reports that for a known TSP problem (pr1002 of the TSPLIB), quantum annealing shows significant improvements in run time over simulated annealing. While the authors acknowledge that TSP-specific algorithms still perform better than simulated or quantum annealing, they believe that as a general optimization algorithm, quantum annealing shows potential for speed ups [10].

4 D-Wave

Now let's examine a specific implementation of a quantum annealer. D-Wave Systems is a company founded in 1999 specializing in the commercialization of quantum annealing. In 2011, the company introduced their first machine, a 128-qubit annealer called the D-Wave One. This was followed by a 1000+ qubit machine, the D-Wave 2X in 2015. In 2020, the company launched it's Leap cloud computing service with a 5000+ qubit system.

D-Wave machines use superconducting qubits in their quantum processor unit (QPU). In order to implement the time-Hamiltonian that we wish to anneal (equation 3.2) the D-Wave system uses [11],

1. A global field (x-direction) to generate the transverse field term. This term is slowly reduced throughout the annealing process.
2. Magnetic biases (z-direction) to generate the external field terms h_i in the Ising Hamiltonian.
3. Devices called couplers to generate entanglement between qubits and resulting in the interaction terms J_{ij} in the Ising Hamiltonian.

4.1 D-Wave Controversy

While D-Wave technologies seem to show a lot of promise, they have also been subject to many controversies. In 2013, physicists in the field expressed concern that the D-Wave One's qubits exhibit large decoherences. This may suggest that the D-Wave One can not effectively harness quantum phenomena and instead operates as a thermal annealer. As a further challenge, the dissenters showed that D-Wave's own proof of quantumness can be consistent with classical behavior [12].

Another notable example, in 2015 D-Wave published findings that their machine could solve a series of problems faster than classical algorithms by a factor of 10^8 [13]. However, further articles dispute their claim, indicating that D-Wave's benchmark problems can be solved exactly and in polynomial time via classical algorithms the company failed to mention [14].

5 Discussion

In this section, we'll briefly address some common questions and distinctions regarding quantum annealing.

5.1 Why the Ising model?

The subset of problems that can be tackled with quantum annealing is strictly restricted to those that can be mapped to an Ising Hamiltonian. Why is this the case and why do we choose the Ising Hamiltonian?

Practically, we choose to reduce the type of Hamiltonian that we can anneal to Ising Hamiltonian because it is simple to implement (with system like D-Wave) compared to an arbitrary Hamiltonian. Furthermore, while an Ising Hamiltonian does provide restrictions, a wide variety of problems, including graph problems such as TSP, can be mapped to the Ising model. Thus, quantum annealing is still relatively versatile.

5.2 Quantum Annealing versus Adiabatic Quantum Computation

The primary distinction between quantum annealing and adiabatic quantum computation is the type of Hamiltonian. While QA is restricted to the Ising Hamiltonian, AQC describes the general technique to find the ground state of an arbitrary Hamiltonian.

Since AQC is must less restrictive on the problem type, it can be shown that any collection of unitary operations can be mapped in polynomial time to annealing a Hamiltonian [9]. Thus, unlike QA, AQC is classified as a universal quantum computer.

5.3 Adiabatic Computing versus the Circuit Model

Quantum annealing is an exciting prospect in the near-term because it is relatively "easy" to implement (as exemplified the current state of commercial annealers). But how does current technology compare to a fully-realized gate-model quantum computer?

Since quantum annealing is not a universal technique, we would expect the circuit model to dominate. However, in comparing AQC with the circuit model, is very feasible that AQC can excel in certain optimization problem in comparison to equivalent algorithms in the gate-model.

5.4 Conclusion

In summary, quantum annealing is a computation technique that utilizes quantum phenomena to solve combinatorial optimization problems that can be mapped onto the Ising model. As its name suggests, quantum annealers operate on the principle of adiabatic annealing of a problem Hamiltonian. There currently exists implementations of quantum annealing, notably, those produced by the company D-Wave.

While much remains to be done in the field to show efficacy, scalability, and universality of this technology, the continued development of quantum annealing holds significant potential for both near and long-term quantum computation.

References

[1] M. Vogel, *Quantum Computation and Quantum Information, by M.A. Nielsen and I.L. Chuang*, vol. 52. 2011.

[2] C. A. Pérez-Delgado and P. Kok, "Quantum computers: Definition and implementations," *Physical Review A - Atomic, Molecular, and Optical Physics*, vol. 83, no. 1, pp. 1–15, 2011.

[3] A. Das and B. K. Chakrabarti, "Colloquium: Quantum annealing and analog quantum computation," *Reviews of Modern Physics*, vol. 80, no. 3, pp. 1061–1081, 2008.

[4] M. Vafaei Jahan and M. R. Akbarzadeh-T, "Extremal optimization vs. learning automata: Strategies for spin selection in portfolio selection problems," *Applied Soft Computing Journal*, vol. 12, no. 10, pp. 3276–3284, 2012.

[5] G. H. Sasaki and B. Hajek, "The time complexity of maximum matching by simulated annealing," *Journal of the ACM (JACM)*, vol. 35, no. 2, pp. 387–403, 1988.

[6] S. Geman and D. Geman, "Stochastic Relaxation, Gibbs Distributions, and the Bayesian Restoration of Images," *IEEE Transactions on Pattern Analysis and Machine Intelligence*, vol. PAMI-6, no. 6, pp. 721–741, 1984.

[7] D. Bertsimas and J. Tsitsiklis, "Simulated annealing," *Statist. Sci.*, vol. 8, pp. 10–15, 02 1993.

[8] M. H. Amin, "Consistency of the adiabatic theorem," *Physical review letters*, vol. 102, no. 22, p. 220401, 2009.

[9] T. Albash and D. A. Lidar, "Adiabatic quantum computation," *Reviews of Modern Physics*, vol. 90, no. 1, 2018.

[10] R. Martoňák, G. E. Santoro, and E. Tosatti, "Quantum annealing of the traveling-salesman problem," *Physical Review E - Statistical Physics, Plasmas, Fluids, and Related Interdisciplinary Topics*, vol. 70, no. 5, p. 4, 2004.

[11] D.-W. S. Documentation, *What is Quantum Annealing?*

[12] J. A. Smolin and G. Smith, "Classical signature of quantum annealing," *Frontiers in Physics*, vol. 2, pp. 1–5, 2014.

[13] V. S. Denchev, S. Boixo, S. V. Isakov, N. Ding, R. Babbush, V. Smelyanskiy, J. Martinis, and H. Neven, "What is the computational value of finite-range tunneling?," *Physical Review X*, vol. 6, no. 3, pp. 1–19, 2016.

[14] S. Mandrà, H. G. Katzgraber, and C. Thomas, "The pitfalls of planar spin-glass benchmarks: Raising the bar for quantum annealers (again)," *arXiv*, 2017.

[15] A. Das and B. Chakrabarti, *Quantum Annealing and Related Optimization Methods*. No. August, 2014.

[16] E. Farhi, J. Goldstone, S. Gutmann, and M. Sipser, "Quantum Computation by Adiabatic Evolution," 2000.

[17] R. Harris, M. W. Johnson, T. Lanting, A. J. Berkley, J. Johansson, P. Bunyk, E. Tolkacheva, E. Ladizinsky, N. Ladizinsky, T. Oh, F. Cioata, I. Perminov, P. Spear, C. Enderud, C. Rich, S. Uchaikin, M. C. Thom, E. M. Chapple, J. Wang, B. Wilson, M. H. Amin, N. Dickson, K. Karimi, B. MacReady, C. J. Truncik, and G. Rose, "Experimental investigation of an eight-qubit unit cell in a superconducting optimization processor," *Physical Review B - Condensed Matter and Materials Physics*, vol. 82, no. 2, pp. 1–15, 2010.

[18] I. Introduction, "Thermodynamical Approach to the Traveling Salesman Problem : An Efficient Simulation Algorithm I," vol. 45, no. l, pp. 41–51, 1985.

[19] T. Kadowaki and H. Nishimori, "Quantum annealing in the transverse Ising model," vol. 58, no. 5, pp. 5355–5363, 1998.

[20] T. Review, "Optimization using quantum mechanics : quantum annealing through adiabatic evolution Optimization using quantum mechanics : quantum," 2006.

[21] R. D. Somma, D. Nagaj, and M. Kieferová, "Quantum speedup by quantum annealing," *Physical Review Letters*, vol. 109, no. 5, pp. 1–5, 2012.

[22] R. H. Warren, "Solving the traveling salesman problem on a quantum annealer," *SN Applied Sciences*, vol. 2, no. 1, pp. 1–5, 2020.