Quantum annealing for problems with ground-state degeneracy

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Abstract. We study the performance of quantum annealing for systems with ground-state degeneracy by directly solving the Schrödinger equation for small systems and quantum Monte Carlo simulations for larger systems. The results indicate that quantum annealing may not be well suited to identify all degenerate ground-state configurations, although the value of the ground-state energy is often efficiently estimated. The strengths and weaknesses of quantum annealing for problems with degenerate ground states are discussed in comparison with classical simulated annealing.

1. Introduction

Quantum annealing (QA) \([1, 2]\) is the quantum-mechanical version of the simulated annealing (SA) \([3]\) algorithm to study optimization problems. While the latter uses the slow annealing of (classical) thermal fluctuations to obtain a ground-state estimate, the former uses quantum fluctuations. An extensive body of numerical \([4, 5, 6, 7]\) as well as analytical \([8]\) studies show that QA is generally more efficient than SA for the ground-state search (optimization) of classical Hamiltonians of the Ising type. This fact does not immediately imply, however, that SA will soon be replaced by QA in practical applications because the full implementation of QA needs an efficient method for solving the Schrödinger equation for large systems, a task optimally achievable only on quantum computers. Given continuing progress in the implementability of quantum computers, we thus continue to study the theoretical efficiency and the limit of applicability of QA using small-size prototypes and classical simulations of quantum systems, following the general spirit of quantum information theory.

The present paper is a partial report on these efforts with a focus on the efficiency of QA when the ground state of the studied model is degenerate, i.e., when different configurations of the degrees of freedom yield the same lowest-possible energy. So far, almost all problems studied with QA have been for nondegenerate cases, and researchers have not paid particular attention to the role played by degeneracy. This question, however, needs careful scrutiny because many practical problems have degenerate ground states.

If the goal of the minimization of a Hamiltonian (cost function) of a given problem is to obtain the ground-state energy (minimum of the cost function), it suffices to reach one of the degenerate ground states, which might often be easier than an equivalent nondegenerate problem because there are many states that are energetically equivalent. If, on the other hand, we are asked to identify all (or many of) the degenerate ground-state configurations (arguments of the cost function which minimize it) and not just the lowest value of the energy, we have to carefully
check if all ground states can be found. This would thus mean that the chosen algorithm can reach all possible ground-state configurations ergodically. Such a situation would happen if, for instance, we want to compute the ground-state entropy or we may need the detailed spin configuration of a spin-glass system to understand the relationship between the distribution of frustration and the ground-state configurations.

We have investigated this problem for a few typical systems with degeneracy caused by frustration effects in the interactions between Ising spins. Our results indicate that QA is not necessarily well suited for the identification of all the degenerate ground states, i.e., the method fails to find certain ground-state configurations independent of the annealing rate. This is in contrast to SA, with which all the degenerate states are reached with almost equal probability if the annealing rate of the temperature is sufficiently slow. Nevertheless, when only the ground-state energy is needed, QA is found to be superior to SA in some example systems.

The present paper is organized as follows: Section 2 describes the solution of a small system by direct diagonalization and numerical integration of the Schrödinger equation. Section 3 is devoted to the studies of larger degenerate systems via quantum Monte Carlo simulations, followed by concluding remarks in section 4.

2. Schrödinger dynamics for a small system

It is instructive to first study a small-size system by a direct solution of the Schrödinger equation, both in stationary and nonstationary contexts. The classical optimization problem for this purpose is chosen to be a five-spin system with interactions as shown in figure 1.

![Figure 1. Five-spin toy model studied. Full lines denote ferromagnetic interactions \( J_{ij} = 1 \) while dashed lines stand for antiferromagnetic interactions \( J_{ij} = -1 \). Because of the geometry of the problem the system has a degenerate ground state by construction.](image)

The Hamiltonian of this system is given by

\[
H_0 = - \sum_{\langle ij \rangle} J_{ij} \sigma^z_i \sigma^z_j, \tag{1}
\]

where the sum is over all nearest-neighbor interactions \( J_{ij} = \pm 1 \) and \( \sigma^z_i \) denote Ising spins parallel to the \( z \)-axis. The system has six degenerate ground states, three of which are shown in figure 2. We apply a transverse field

\[
H_1 = - \sum_{i=1}^{5} \sigma^x_i \tag{2}
\]

to the system \( H_0 \) to induce a quantum transition between classical states. The total Hamiltonian \( H(t) \) changes from \( H_1 \) at \( t = 0 \) to \( H_0 \) at \( t = \tau \), i.e.,

\[
H(t) = \left( 1 - \frac{t}{\tau} \right) H_1 + \frac{t}{\tau} H_0. \tag{3}
\]
Figure 2. Nontrivial degenerate ground states of the toy model shown in figure 1. The other three ground states $|\bar{1}\rangle$, $|\bar{2}\rangle$, and $|\bar{3}\rangle$ are obtained from $|1\rangle$, $|2\rangle$, and $|3\rangle$ by reversing all spins.

For large $\tau$ the system is more likely to follow the instantaneous ground state according to the adiabatic theorem. If the target optimization Hamiltonian $H_0$ had no degeneracy in the ground state, the simple adiabatic evolution ($\tau \gg 1$) would drive the system from the trivial initial ground state of $H_1$ to the nontrivial final ground state of $H_0$ (solution of the optimization problem).

The situation changes significantly for the present degenerate case as illustrated in figure 3, which depicts the instantaneous energy spectrum. Some of the excited states reach the final ground state as $t/\tau \to 1$. In particular, the instantaneous ground state configurations have been found to be continuously connected to a special symmetric combination of four of the final ground states at $t = \tau$, $|2\rangle + |\bar{2}\rangle + |3\rangle + |\bar{3}\rangle$, whereas the other two states $|1\rangle$ and $|\bar{1}\rangle$ are out of reach as long as the system faithfully follows the instantaneous ground state ($\tau \gg 1$). A relatively quick time evolution with an intermediate value of $\tau$ may catch the missed ground states. However, there is no guarantee that the obtained state using this procedure is a true ground state since one of the final excited states may be reached. As shown in the left panel of figure 4, intermediate values of $\tau$ around 10 give almost an even probability to all the true ground states, an ideal situation. However, the problem is that we do not know an appropriate value of $\tau$ beforehand. In contrast, the right panel of figure 4 shows the result of SA by a direct numerical integration of the master equation, in which all the states are reached evenly in the limit of large $\tau$. Figure 3 suggests that it might be plausible to start from one of the low-lying excited states of $H_1$ to reach the missed ground state. However, such a process has also been found to cause similar problems as above. We therefore conclude that QA is not suitable to find all degenerate ground-state configurations of the target system $H_0$, at least in the present example. This aspect is to be contrasted with SA, in which infinitely-slow annealing of the temperature certainly finds all ground states with equal probability as assured by the theorem of Geman and Geman [9].

Figure 3. Instantaneous energy spectrum of the five-spin system depicted in figure 1. For simplicity we have omitted the energy levels that are not reachable from the ground state due to different symmetry properties.
Figure 4. Annealing-time dependence of the final probability that the system is in any one of the ground states. Left panel: Data for the five-spin model using QA. Only the states $|2\rangle$ and $|3\rangle$ (and their reversals $|\bar{2}\rangle$ and $|\bar{3}\rangle$) are reached for large $\tau$. Right panel: In contrast, SA finds all the states with equal probability.

QA nevertheless shows astounding robustness against a small perturbation that lifts part of the degeneracy if our interest is in the value of the ground-state energy. Figure 5 depicts the residual energy—the difference between the obtained approximate energy and the true ground-state energy—as a function of the annealing time $\tau$. Data using SA are also shown in figure

Figure 5.
Residual energy per spin as a function of the annealing time $\tau$ for the five-spin toy model. Left panel: Degenerate case. Right panel: A small perturbation $h = 0.10$ [see equation (4)] has been added to lift the overall spin-reversal symmetry and thus break the degeneracy. While QA is rather robust against the inclusion of a field term and the residual energy per spin decays in both cases $\sim \tau^{-2}$ for large $\tau$, SA seems not to converge after the inclusion of a field term. Dotted lines represent the results in zero field for comparison.

5 using an annealing schedule of temperature $T = (\tau - t)/t$, corresponding to the ratio of the first and the second terms on the right-hand side of equation (3). In the degenerate case (left panel) it seems that SA outperforms QA since the residual energy decays more rapidly using
SA. However, if we apply a small longitudinal field to $H_0$

$$H_2 = -h \sum_{i=1}^{5} \sigma_i^z$$

and regard $H_0 + H_2$ as the target Hamiltonian to be minimized, the situation changes drastically: The convergence of SA slows down significantly while the convergence of QA remains almost intact (right panel of figure 5). As already observed in the simple double-well potential problem [10], the energy barrier between the two almost degenerate states of $H_0 + H_2$ may be too high to be surmountable by SA whereas the width of the barrier remains thin enough to allow for quantum tunnelling to keep QA working.

3. Monte Carlo simulations for larger systems

The simplest Ising model which possesses an exponentially-large (in the system size) ground-state degeneracy is the two-dimensional Villain fully-frustrated Ising model [11]. The Ising model is defined on a square lattice of size $N = L \times L$ and has alternating ferromagnetic and antiferromagnetic interactions in the horizontal direction and ferromagnetic interactions in the vertical direction; see figure 6. We use periodic boundary conditions and show data for $L = 6$ with $M = 1/T = 100$, where $M$ is the number of Trotter slices and $T$ the temperature. We first pre-anneal the system by decreasing the temperature as $T = 100/Mt$ from $t = 0$ to 100 and then decrease the transverse field by the schedule $\Gamma = (\tau - t)/t$ from $t = 0$ to 100 (after resetting $t$ to 0) with $T$ fixed.

![Figure 6. Fully-frustrated Ising model with $N = 36$ spins (dots) and periodic boundary conditions. The system has 45088 degenerate ground states (excluding spin-reversal symmetry). The horizontal bonds alternate between ferromagnetic (full lines) and antiferromagnetic (dashed lines). The vertical bonds are all ferromagnetic. This ensures that the product of all bonds around any plaquette is negative, i.e., the system is maximally frustrated.](image)

The left panel of figure 7 shows a linear-log plot of the relative number of ground-state hits versus the ground-state numbering (sorted by the number of hits). While a small part of the total set of ground states are reached very frequently, some ground states seem exponentially suppressed. Furthermore, this seems almost independent of the chosen value of the annealing time $\tau$ in the Monte Carlo simulation. In the right panel of figure 7 we show the relative number of ground-state hits versus the ground-state numbering for SA. In contrast to QA, SA finds almost all ground states with even probability. While some ground states seem to be preferred, all ground states can be reached with a frequency of at least 40% (see also Ref. [12]). The residual energy is shown in the left panel of figure 8. The data for SA follow a rapid decrease beyond $\tau \approx 2 \times 10^3$, whereas QA stays unimproved beyond this region. This saturation may reflect the finiteness of the temperature of QA because we have found that the saturation time (measured in Monte Carlo steps) is larger than $2 \times 10^3$ for smaller $T$ (larger $M$). Note that the energy for QA has been estimated as the average value of energies of all Trotter slices that emerge in the quantum-classical mapping for the quantum Monte Carlo simulation. The best value among the Trotter slices shows better performance. Since we are not certain if such a process constitutes a fare comparison with SA, we avoid further details here.
**Figure 7.** Histograms of the relative frequency that a given ground state is reached by QA (left panel) and SA (right panel). In the abscissa the ground states are numbered according to their relative frequency to be reached, and thus the histograms are monotonically decreasing. While SA finds most ground states evenly and all ground states can be reached at least 40% of the time, in QA some ground states seem exponentially suppressed.

**Figure 8.** Left panel: Residual energy per spin for the fully-frustrated Ising model with $L = 40$ using QA and SA. While the residual energy per spin for SA decreases monotonically, for QA it saturates around $\tau \approx 2 \times 10^3$. Right panel: Residual energy per spin for the $\pm J$ Ising spin glass with $L = 40$. QA shows a more rapid decay than SA both in the sample average and minimum value between samples.

Finally, we also show some preliminary data for the two-dimensional bimodal ($\pm J$) Ising spin glass [13]. In this case the situation is quite different, as can be seen in the right panel of figure 8. The residual energy using QA decreases more rapidly than when using SA. For this particular model it seems that QA is a powerful tool, as witnessed in previous studies [1, 4, 5, 6].

### 4. Conclusion
We have studied the performance of QA for systems with degeneracy in the ground state of the target Hamiltonian. Our results show that QA reaches only a limited part of the set of
degenerate ground-state configurations and misses the other states. The instantaneous energy spectrum as a function of time, figure 3, is a useful tool to understand the situation: some of the excited states merge to the final ground states as $t/\tau \rightarrow 1$. It is usually difficult, however, to initially select the appropriate excited states which reach the ground state when $t/\tau \rightarrow 1$. We therefore have to be biased a priori in the state search by QA for degenerate cases. Simulations on nontrivial Ising models with ground-state degeneracy such as the two-dimensional Villain model show that certain ground-state configurations are exponentially suppressed when using QA, whereas this is not the case when using SA. Nevertheless, if the problem is to find the ground-state energy, QA is often (but not necessarily always) an efficient method as exemplified in figure 5 where the residual energies are shown. It is clearly necessary to study more examples and to construct an analytical theory based on the numerical evidence to establish criteria when to (and when not to) use QA.

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