

# D-Wave 3-qubit Problem

Nicholas Ezzell \*

Quantum Computing Division, Oak Ridge National Lab

(Dated: July 13, 2018)

I was going to send this information over email, but I figured it would be easier to communicate if I just made a L<sup>A</sup>T<sub>E</sub>X document. The figures are pdfs, as I wanted it be possible for you to view them as is as well, but this means they are poorly formatted for L<sup>A</sup>T<sub>E</sub>X, but that's okay; I'll make them better whenever I have to write the final report.

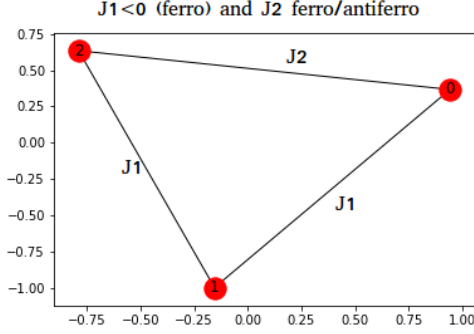


FIG. 1. Coupling strength  $J1$  between qubits (0, 1) and (1, 2) represents a ferromagnetic “nearest-neighbor” interactions. Coupling strength  $J2$  between qubits (0, 2) can be ferromagnetic or anti-ferromagnetic and represents “next-nearest-neighbor” interactions.

## INTRODUCTION

We wish to use D-Wave to simulate quantum phase transitions on the simple 3-qubit triangular lattice shown in Fig. 1.

## PHASE-DIAGRAMS

In this context, the word “phase” is used loosely to mean the probability that the ground state of the 3 qubit system for a given set of coupling and field-bias strengths is ferromagnetic.

## Numeric Calculations

We will begin by showing the resulting phase diagrams generated by solving this problem numerically with Mathematica. The procedure was as follows: diagonalize  $H$  for given  $J1$ ,  $J2$ , and  $h$ , obtain ground-state, and find the ratio of ground-states that are ferromagnetic to non-ferromagnetic.

Note: Since the legends got cut-off, note that violet = 0% chance of being ferromagnetic and red is 100% chance where gradient is ROYGBIV.

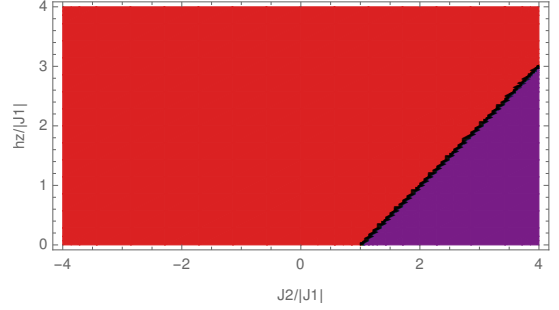


FIG. 2. Probability that the ground state of 3 qubit system is ferromagnetic for a given set of  $J1$ ,  $J2$ , and  $h$ —the strength of the qubit’s coupling to a longitudinal magnetic field. Computation done numerically with Mathematica.

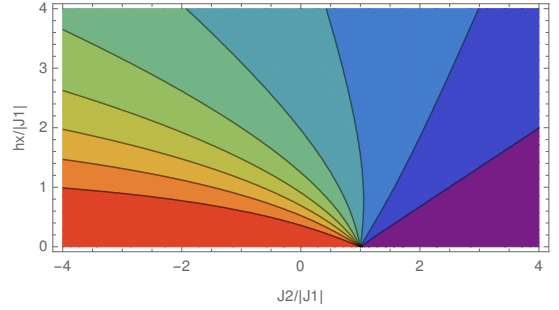


FIG. 3. Probability that the ground state of 3 qubit system is ferromagnetic for a given set of  $J1$ ,  $J2$ , and  $h$ —the strength of the qubit’s coupling to a transverse magnetic field. Computation done numerically with Mathematica.

*Longitudinal Field*

*Transverse Field*

I am fairly confident in these numeric results, as the transverse field plot matches that as seen in Edwards [1]. While I don’t know of any papers that show the longitudinal plot, I used the same numeric process, and my D-Wave results match the longitudinal plot.

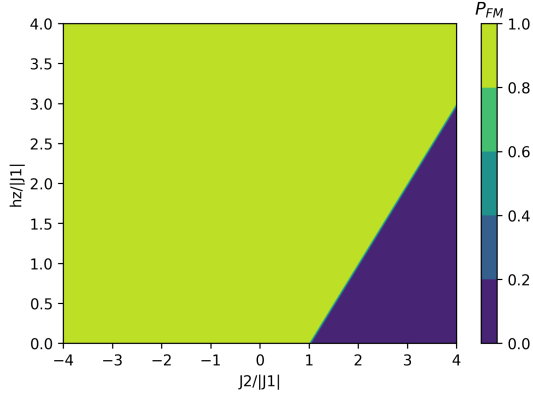


FIG. 4. Probability that the ground state of 3 qubit system is ferromagnetic for a given set of  $J1$ ,  $J2$ , and  $h$ —the strength of the qubit’s coupling to a longitudinal magnetic field. Simulation done with D-Wave 2000Q-2 chip.

### D-Wave Simulations

Now we will produce the same phase-diagrams produced by simulating the 3 qubit problem on the D-Wave. Doing so, however, requires consideration of several factors such as

1. the *Minor-embedding*
2. the *Anneal schedule*
3. and potential *Chip errors*.

#### Longitudinal Field

The D-Wave simulations match the numeric calculations well as shown in Figures 2 and 4. In regards to the above considerations, the following can be said:

1. D-Wave’s CMR [2] default embedding algorithm is sufficient to produce these results, but a self-created square embedding also worked.
2. The default annealing time of  $20\mu s$  was sufficient, though later results indicate that the same results could be obtained with an anneal faster than this.
3. Since this is a small problem, anneal time was sufficiently long. Furthermore, finite-temperature errors were mitigated by only accepting lowest energy states for a given run (in batches of 246). Finally, “innate” chip couplings did not passively affect the results, as tiling 246 instances of the problem on the chip at a time versus running the singular problem many times produces the same results.

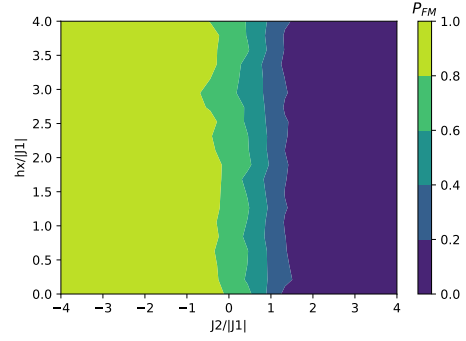


FIG. 5. Probability that the ground state of 3 qubit system is ferromagnetic for a given set of  $J1$ ,  $J2$ , and  $h$ —the strength of the qubit’s coupling to a transverse magnetic field. Computation done numerically with Mathematica.

#### Transverse Field

The D-Wave simulations do not match the numeric calculations very well as shown in Figures 3 and 5. In regards to the above considerations, (1) and (3) are mostly met by virtue of being met for the Longitudinal model with the exception of culling the higher energy states. Here, all states must be kept since the ground state of the transverse Hamiltonian has uncertainty in the energy with respect to the computational basis. Thus, it is likely that (2) is the source of the error, as transverse-field terms are introduced by manipulating the `anneal_schedule` parameter passed to the chips.

Note: This newest contour plot with my new API makes more sense than the last one wherein the violet line was present at the top of the plot rather than on the right. I believe this resulted from a minor bug where I associated the wrong  $p_{FM}$  with a given set of  $J1$ ,  $J2$ , and  $h$ . Here, at least an anti-ferromagnetic  $J2$  still gives rise to little to no probability of getting a ferromagnetic ground-state.

### IDENTIFYING THE SOURCE OF TRANSVERSE-FIELD SIMULATION ERROR

To understand what caused the discrepancy between the numeric calculations and the D-Wave simulation, I extended the functionality of my Mathematica calculations and improved the post-processing utilities of my simulation framework. To understand exactly what I did, one must first understand what “anneal scheduling” means on the D-Wave machine.

In general, any quantum annealing algorithm works by transforming some initial Hamiltonian,  $H_I$  to some final Hamiltonian,  $H_F$ . On the D-Wave, this procedure takes

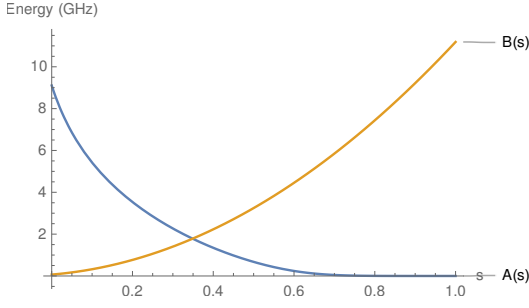


FIG. 6. The  $A(s)$  and  $B(s)$  functions.

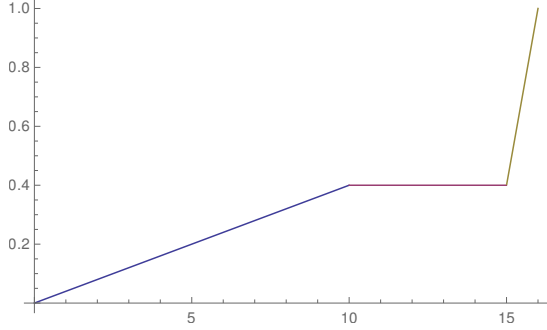


FIG. 7. An example user-defined anneal schedule for a forward anneal. In the terminology of D-Wave, this represents a forward anneal for  $10\mu s$  up to  $s = 0.4$  followed by a  $5\mu s$  pause and a  $1\mu s$  quench. Despite the terminology, all anneal schedules must end with  $s = 1$  and cannot be “stopped early.”

the specific form

$$H(s(t)) = \frac{A(s(t))}{2} \sum_i^N \sigma_i^x + \frac{B(s(t))}{2} \left( \sum_i^N h_i \sigma_i^z + \sum_{i<j}^N J_{ij} \sigma_i^z \sigma_j^z \right), \quad (1)$$

where  $A(s)$  and  $B(s)$  are monotonically decreasing/increasing functions fixed by the hardware (see Fig. 6) with  $A(s) \gg B(s)$  at  $s = 0$  and  $B(s) \gg A(s)$  at  $s = 1$ . Though  $A(s)$  and  $B(s)$  cannot be changed, the rate of change of  $s$  with respect to  $t$  can be user-defined as a collection of up to three(four) connected lines for forward(reverse) annealing (see Fig. 7).

As can be seen in Eq. 1, the only way to introduce transverse-field terms ( $\sigma_x$ ) is to abruptly take a measurement somewhere in the middle of the anneal when  $A(s)$  is non-negligible. Unfortunately, this is not possible, as all anneal schedules must end with  $s = 1$  as shown in the example of Fig. 7. To reconcile these two seemingly mutually exclusive constraints, one must employ the “sudden approximation.” This approximation ensures that if a system’s Hamiltonian is changed from  $H(s')$  to  $H_F$  *fast enough*, then the system will not have time to adjust and

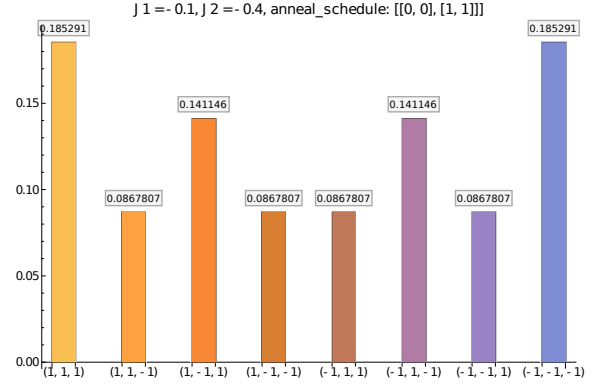


FIG. 8. The distribution of states obtained using a Mathematica annealing simulation of the 3 qubit problem with  $J_1 = -0.1$ ,  $J_2 = -0.4$  and an annealing time of  $1\mu s$ .

be in the same exact state before the rapid change, just written in the new basis of  $H_F$ .

In other words, a transverse field strength  $h_{eff}(s') = \frac{A(s')}{B(s')}$  can be simulated by adiabatically annealing a system to  $s'$  and rapidly finishing the anneal schedule at that point—aka “quenching.” Provided that the quench time,  $t_q$ , is fast with respect to the “system’s dynamics” and the measurement is made at the instant the schedule ends, then the resulting bit-strings will be a reflection of the state of the system at  $s'$  due to the Hamiltonian  $H(s')$ . By sampling over a large number of identical trials, one can reconstruct the original ground-state of  $H(s')$ , getting transverse-Ising model statistics.

### Is the Sudden Approximation Valid?

Given the above discussion, it is natural to ask: just how fast can one quench a problem on the D-Wave? For the 2000Q-2, this corresponds directly to the minimal anneal time of  $1\mu s$ . Okay, great, but is this sufficiently fast with respect to the 3 qubit’s “system dynamics” for the sudden approximation to be valid? My results say no.

### The Numerical Results

To test the validity of the sudden approximation using Mathematica, I simulated a forward anneal of the 3 qubit problem with the D-Wave  $A(s)$  and  $B(s)$  anneal parameters with the minimum anneal time of  $1\mu s$ , getting the distribution of states shown in Figures 8 and 9.

Evidently, the sudden approximation with a  $1\mu s$  anneal time (or quench) is not valid for the 3-qubit problem. Why? If it were, a sudden change from  $H_I$  to  $H_F$  should produce an equal distribution of states, as the initial wave-function is an equal superposition of all pos-

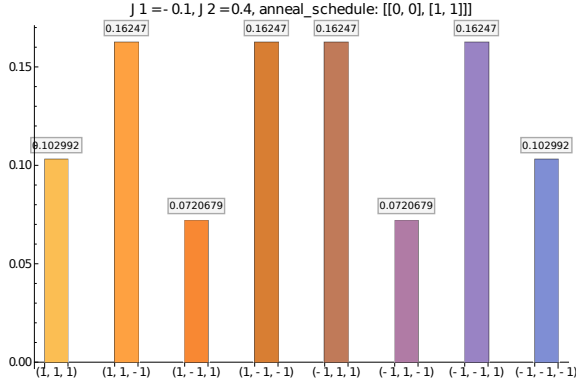


FIG. 9. The distribution of states obtained using a Mathematica annealing simulation of the 3 qubit problem with  $J1 = -0.1$ ,  $J2 = 0.4$  and an annealing time of  $1\mu s$ .

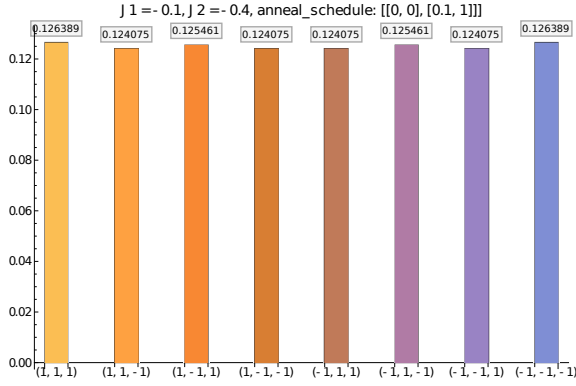


FIG. 10. The distribution of states obtained using a Mathematica annealing simulation of the 3 qubit problem with  $J1 = -0.1$ ,  $J2 = -0.4$  and an annealing time of  $0.1\mu s$ .

sible states in the computational basis. Instead, we get a spread of states where the ground-states of the final Hamiltonian already dominate the output statistics. In order to get an equal distribution of output states, I had to make the anneal time an order of magnitude smaller than  $1\mu s$  down to  $0.1\mu s$ , as seen in Figures 10 and 11.

#### The D-Wave Results

Next, I tried the same test with D-Wave as shown in Figures 12 and 13.

Amazingly, not only is the sudden approximation invalid for the fastest quench on D-Wave (for this 3 qubit problem), it is even more invalid than the Mathematica simulations predict! In order to get similar distribution of states with Mathematica, I had to increase the anneal time by an order of magnitude to  $10\mu s$  as can be seen in Fig 14 and 15.

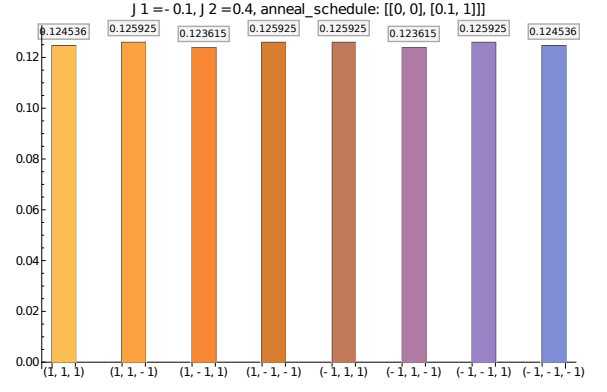


FIG. 11. The distribution of states obtained using a Mathematica annealing simulation of the 3 qubit problem with  $J1 = -0.1$ ,  $J2 = 0.4$  and an annealing time of  $0.1\mu s$ .

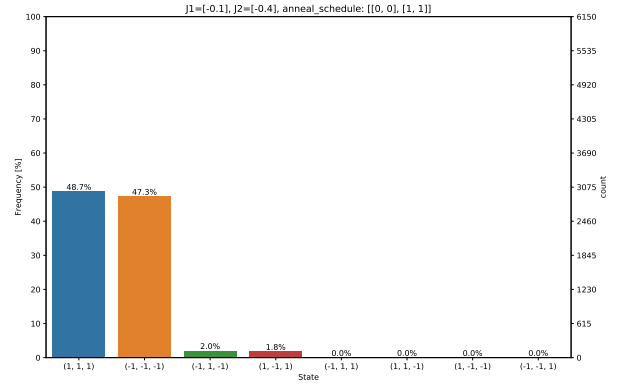


FIG. 12. The distribution of states obtained with a D-Wave simulation of the 3 qubit problem with  $J1 = -0.1$ ,  $J2 = -0.4$  and the minimum annealing time of  $1\mu s$ . It is hard to read, but in essence, the statistics heavily favor the ground-state of the final Hamiltonian, even more so than the numerical simulation of Fig. 8.

## FINAL CONSIDERATIONS

So far, we've learned that the sudden approximation is not valid when annealing from the starting Hamiltonian to the final Hamiltonian with the minimum anneal time possible on the D-Wave chip. Is it conceivable that annealing for a very long time to some  $s'$  over a time  $t_a \gg t_q = 1\mu s$  would reinstate the sudden approximation as valid? From my testing of various more complicated anneal schedules with the same 3 qubit problem the answer is NO. If the sudden approximation is not valid from beginning to end, it cannot be valid in other more contrived anneal schedules for that system. Is it conceivable that the sudden approximation could ever be valid for a system? I suspect the answer is yes, for larger systems where the minimum energy gap grows exponentially small. Why? In this case, the adiabatic theorem predicts

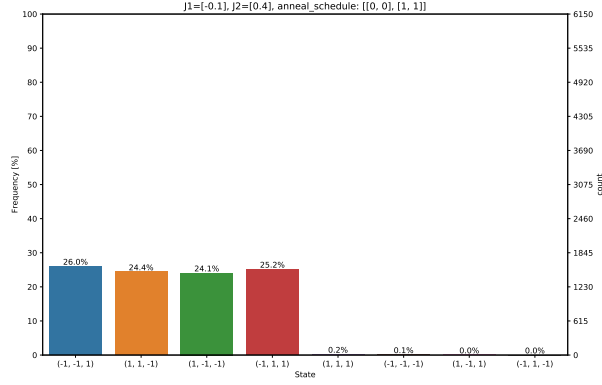


FIG. 13. The distribution of states obtained with a D-Wave simulation of the 3 qubit problem with  $J1 = -0.1$ ,  $J2 = 0.4$  and the minimum annealing time of  $1\mu s$ . It is hard to read, but in essence, the statistics heavily favor the ground-state of the final Hamiltonian, even more so than the numerical simulation of Fig. 9.

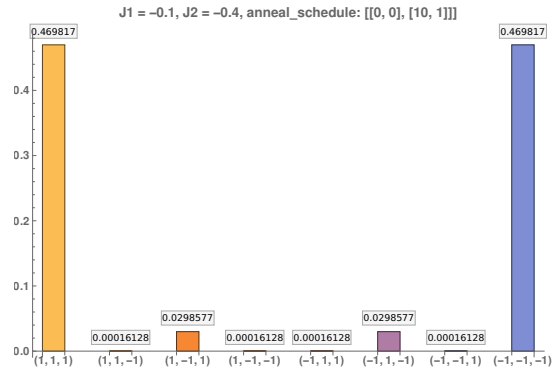


FIG. 14. It takes an anneal time of  $10\mu s$  with the numerical simulation to get the same state statistics that a  $1\mu s$  anneal gives with the D-Wave simulation.

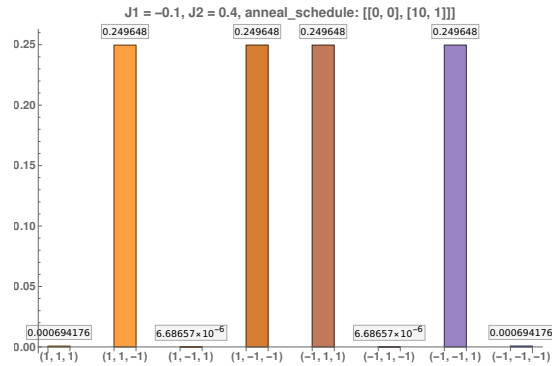


FIG. 15. It takes an anneal time of  $10\mu s$  with the numerical simulation to get the same state statistics that a  $1\mu s$  anneal gives with the D-Wave simulation.

that  $t_a \rightarrow \infty$ , so  $1\mu s \ll t_a$ .

Despite this, we still learned an interesting feature about the chip: it is actually better (in this case) at obtaining the final Hamiltonian's ground-state than the numerical calculations predicted for  $t_a = 1\mu s$ . I think this could be for one of two reasons:

1. The machine is not a perfect closed system at 0K. Additional physics enters the problem than is present in my numerical simulations. Perhaps, this actually helps obtain ground-state statistics in this case, as some open-system papers have predicted/shown for other systems.
2. The measurement of the qubit's states may not happen as the anneal ends. If there is any delay between the ending of the anneal schedule and the measurement, then the system has more time to adjust to the final Hamiltonian than the  $1\mu s$  anneal time leads on.

---

\* Contact Author: nae49@msstate.edu

- [1] Quantum Simulation and Phase Diagram of the Transverse Field Ising Model with Three Atomic Spins
- [2] A practical heuristic for finding graph minors