Using quantum annealing for equilibrium quantum simulation

Vid Eržen
Advisor: Prof. Dr. Dragan Mihailović
Co-advisor: Dr. Jaka Vodeb

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Introduction

1. introduction
2. universality of Ising model
3. quantum annealing
4. equilibrium quantum simulation
5. conclusion

Motivation

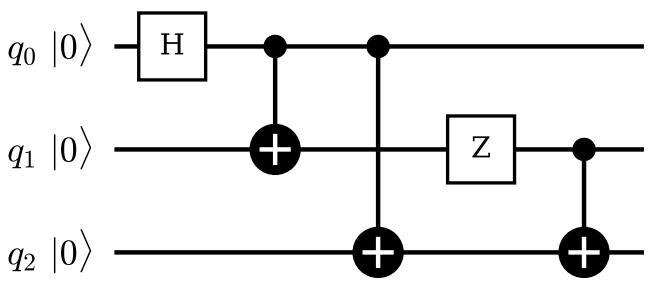
- magnetic phase diagrams in quantum systems
  - Heisenberg model
  - transverse field Ising model (TFIM)
- universal quantum computers currently too small $\rightarrow$ specialized quantum simulators
  - quantum annealing

Quantum annealing and gate model

- computation: programmable transformation input $\rightarrow$ output.

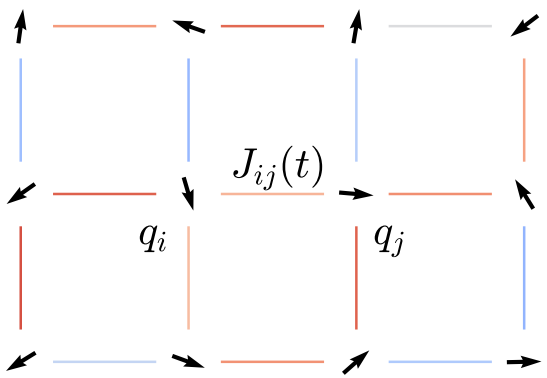
Gate model

- digital (series of quantum gates)
- universal



Quantum annealing

- analog (programmable time-dependent Hamiltonian)
- universality Hamiltonian-dependent



Quantum annealing in practice

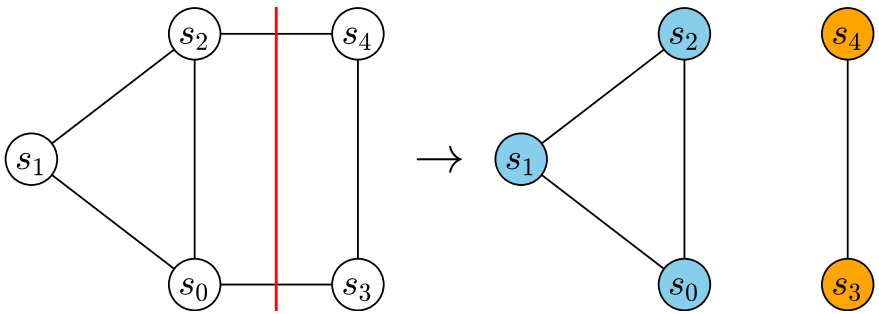
- D-Wave Systems quantum annealers only implement the transverse Field Ising Model (TFIM)

$$H = -\Gamma \sum_i \sigma_i^x + \sum_{\langle i,j \rangle} J_{ij} \sigma_i^z \sigma_j^z + \sum_i h_i \sigma_i^z$$

  - good for optimization problems
  - not general enough for universal quantum computation
  - limited number of simulable physical models
  - quantum Monte Carlo (QMC) methods efficient for equilibrium simulations of TFIM

Optimization problems

- example: graph partitioning problem



1. spin variable $s_i = \begin{cases} 1 & \text{if } i \in A \\ -1 & \text{if } i \in B \end{cases}$
2. minimize number of edges between A and B

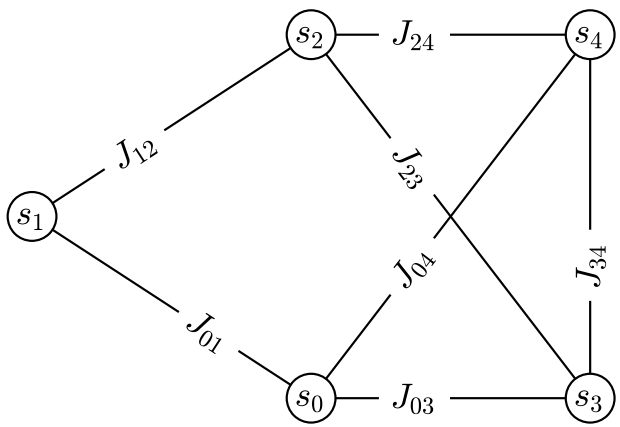
$$H = \sum_{(ij)\in V} \frac{1 - s_i s_j}{2}$$

Universality of Ising model

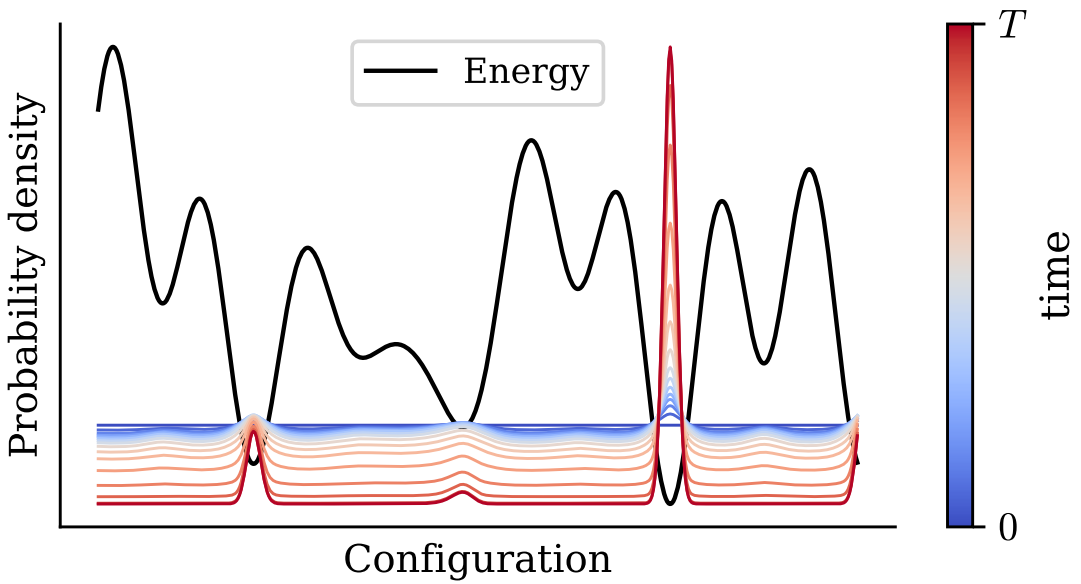
- finding the ground state of an Ising model = solving optimization problems
  - search engine ranking
  - travelling salesman problem
  - scheduling problems

$$H_P = \sum_{i,j} J_{ij} s_i s_j + \sum_i h_i s_i$$

  - J_{ij} and h_i specify the problem
  - $\{s_i = \pm 1\}$ encodes the solution



Can quantum mechanics help us?



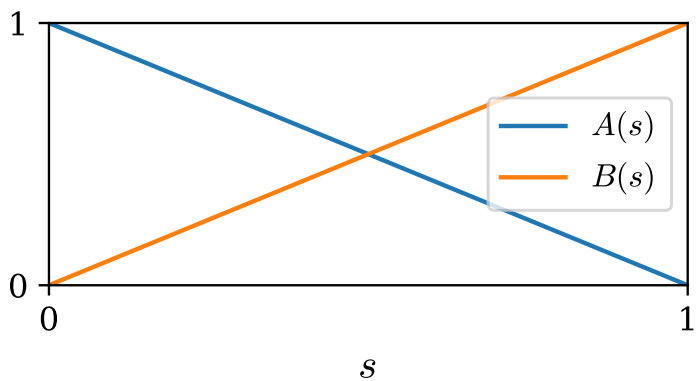
Quantum adabatic theorem

Adiabatic theorem

If a quantum system is prepared in the ground state of a Hamiltonian H_0 and the Hamiltonian is changed slowly enough to H_P, the system will end up in the ground state of H_P.

- interpolating Hamiltonian from H_0 to H_P in time T (dimensionless time $s = t/T$)

$$H(s) = A(s)\, H_0 + B(s)\, H_P$$

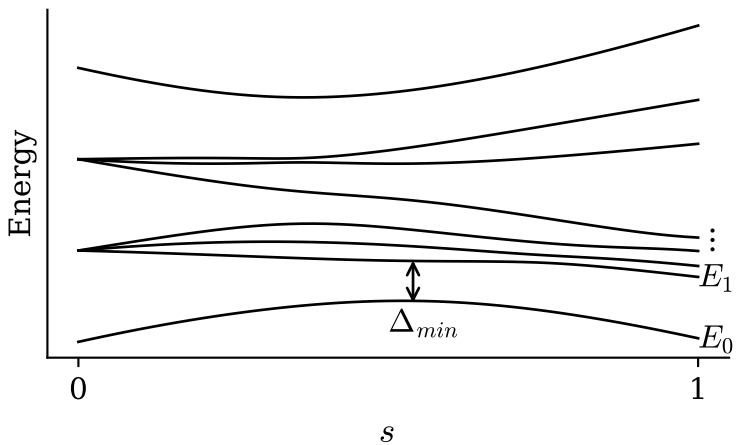


Quantum adiabatic theorem

- interpolating Hamiltonian ($s = t/T$):

$$H(s) = A(s)\, H_0 + B(s)\, H_P$$

- adiabatic theorem, specifically ($\hbar = 1$)



$$T \gg \max_{0 \le s \le 1} \frac{\left| \langle 1(s) | \frac{\partial H}{\partial s} | 0(s) \rangle \right|}{\Delta(s)^2} \implies \left| \langle 0(s=1) | \psi(s=1) \rangle \right|^2 \approx 1$$

Initial Hamiltonian

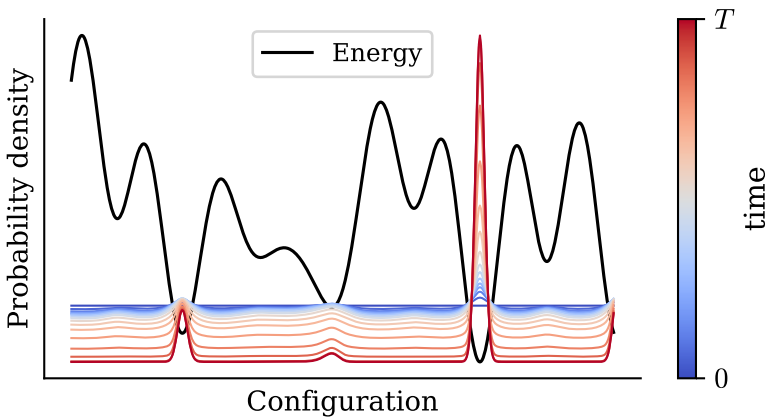
- requirements:
  - operates on two-state quantum systems — qubits
  - easy to prepare its ground state experimentally
  - must not commute with $H_P = \sum_{\langle i,j \rangle} J_{ij}\sigma_i^z\sigma_j^z + \sum_i h_i\sigma_i^z$

- transverse field Hamiltonian

$$H_0 = -\sum_i \sigma_i^x$$

  - ground state

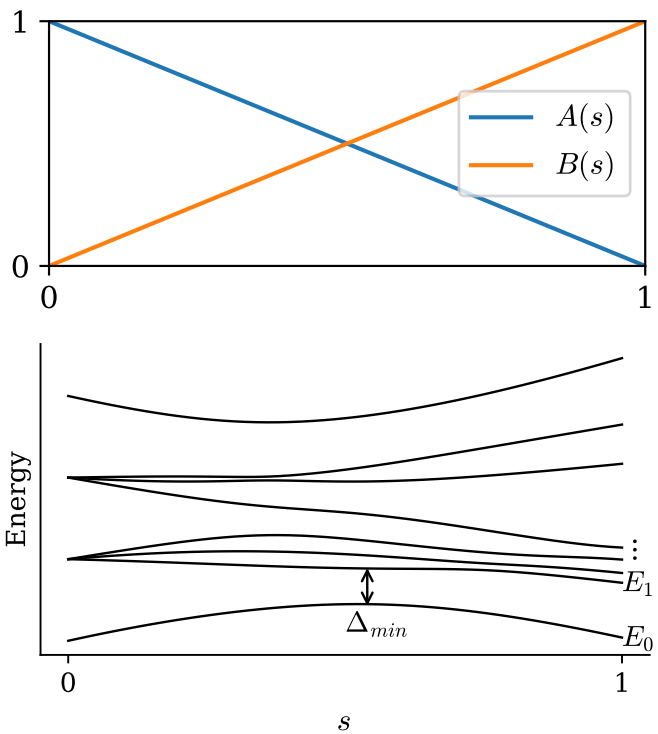
$$|+++...\rangle = \Pi_i^N \frac{|0\rangle_i + |1\rangle_i}{\sqrt{2}}$$

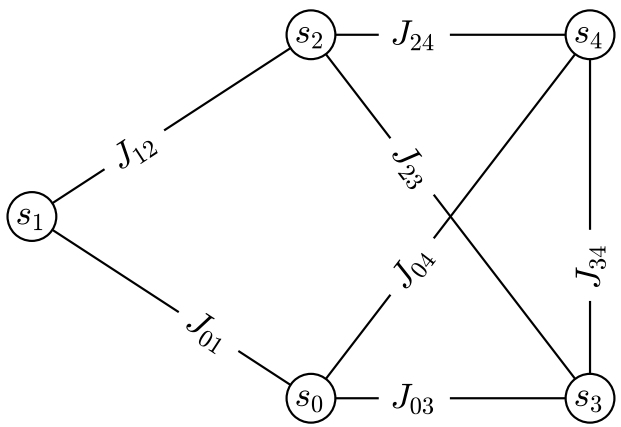


Annealing Hamiltonian

- full quantum annealing Hamiltonian = transverse field Ising model (TFIM)

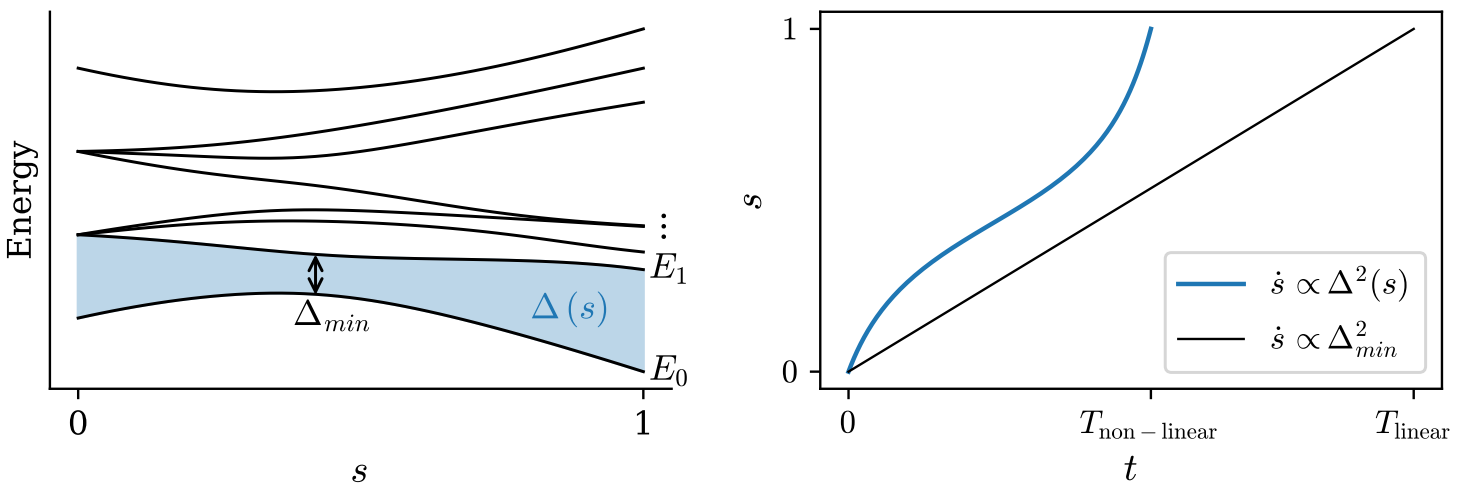
$$H(s) = -A(s)\sum_i \sigma_i^x + B(s)\left(\sum_i h_i\sigma_i^z + \sum_{i,j} J_{ij}\sigma_i^z\sigma_j^z\right)$$





Annealing schedule

- adiabatic theorem: proceed slowly when the gap is small and quickly when the gap is large
  - $s = t/T \rightarrow$ customizable function $s(t)$ (annealing schedule)



Overview

- solving optimization problems = finding the ground state of an Ising model
  - $\{J_{ij}, h_i\}$ specify the problem
- annealing Hamiltonian = Ising + transverse field
  - parts must not commute $\rightarrow$ transitions between states
  - initial ground state as simple as possible

$$H(s) = -A(s)\sum_i \sigma_i^x + B(s)\left(\sum_i h_i\sigma_i^z + \sum_{i,j} J_{ij}\sigma_i^z\sigma_j^z\right)$$

- customizable annealing schedule $s(t)$

Equilibrium quantum simulation

- phase diagram: How does a system behave at different parameters?
  - temperature T
  - magnetic field h_i
  - transverse field $A(s)$
- system with eigenstates $\{|\psi_n\rangle\}$ and eigenenergies $\{E_n\}$ at temperature T

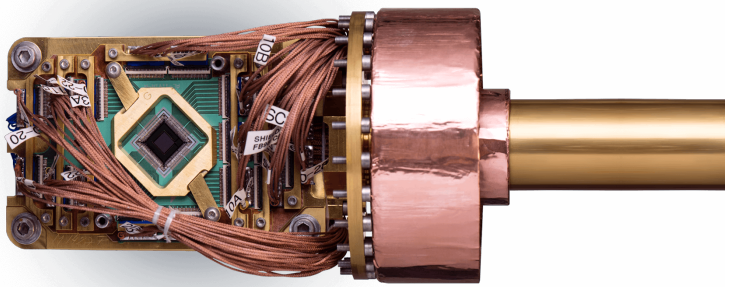
$$p_i = e^{-E_i/T}/Z \tag{1}$$

- Monte Carlo methods: draw N samples $\{s_i\}$ from (1) and estimate observable O

$$\langle O\rangle := \sum_i p_i \langle\psi_i|O|\psi_i\rangle \underset{N\to\infty}{\approx} \frac{1}{N}\sum_{n=1}^{N} O(s_n)$$

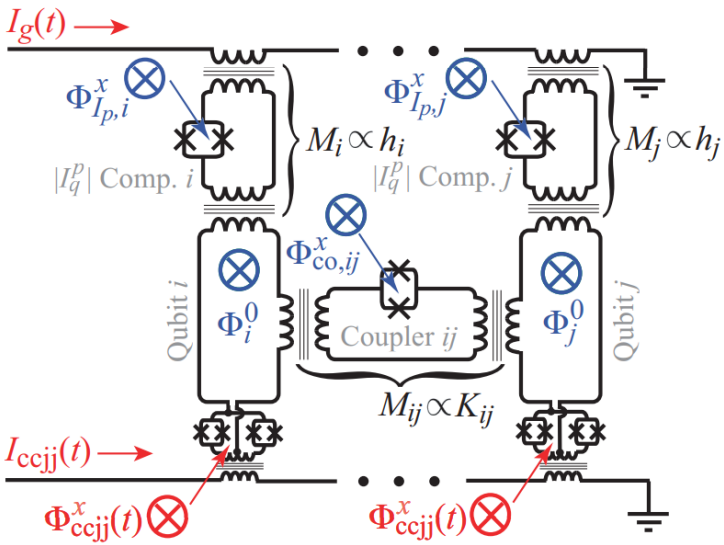
Physical implementation of quantum annealers

- isolated systems
  - deterministic evolution
  - no temperature!
- physical devices couple with their environment at temperature T
  - system thermalizes to T



https://quantumzeitgeist.com

- D-Wave: superconducting qubits in a dilution refrigerator at $T \approx 15\,\mathrm{mK}$



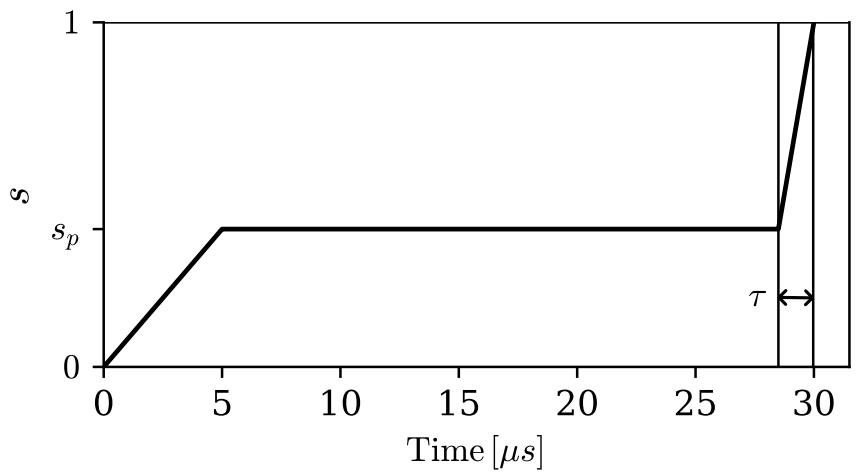
Harris, R. et al. Phys. Rev. B (2010)

Sampling on quantum annealers

- sampling workflow
  1. specify the problem
     - TFIM on the cubic lattice with $J_{ij} = J$ and $h_i = 0$
  2. specify simulation parameters $T, A(s)/B(s)$
  3. map simulation parameters to programmable parameters J, s
  4. embed the lattice onto the hardware graph
  5. obtain samples from the quantum annealer

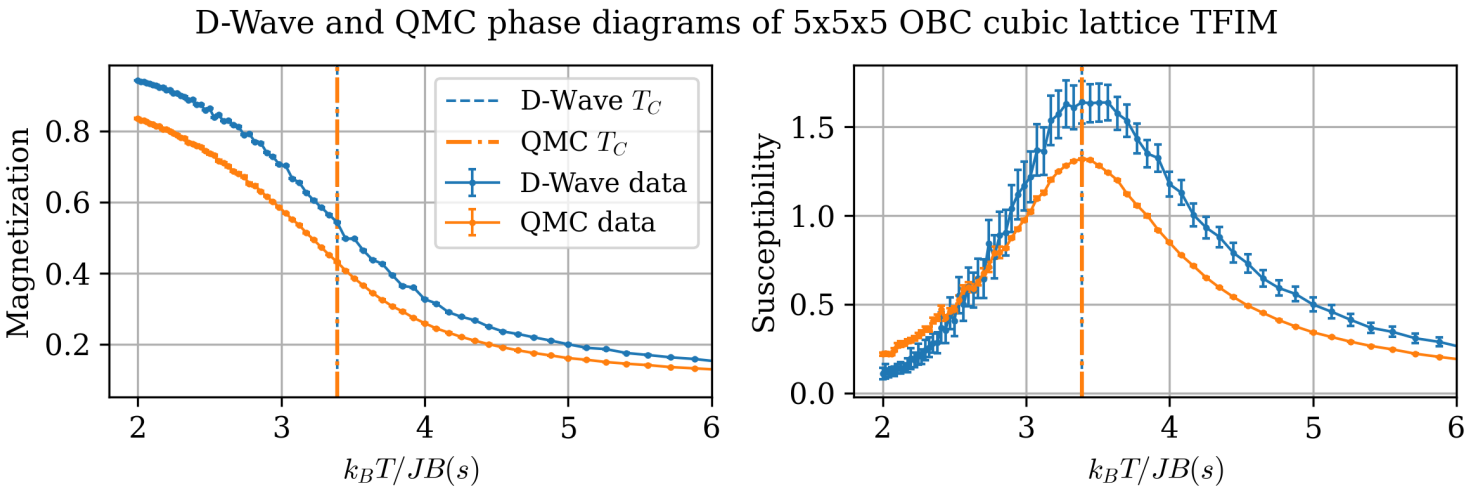
Pause annealing schedule

- protocol for drawing samples from the Boltzmann distribution on quantum annealers
- quench too slow
  - $E\tau/\hbar \sim 10^3$
  - overestimation of magnetization



Magnetization overestimation

- information about the slow quench imprinted in the samples



Quantum Monte Carlo

- do annealers offer an advantage over classical methods?
- quantum Monte Carlo (QMC) methods: TFIM in d dimensions $=$ classical Ising model in $d+1$ dimensions
  - use Metropolis algorithm in $d+1$ dimensions
- TFIM is *stoquastic* (stochastic + quantum)
  - no negative transition probabilities between basis states $|000...\rangle, |100...\rangle, |010...\rangle, \ldots \implies$ TFIM simulable by a stochastic process
- increase the computational power of QA by adding $\sigma^x\sigma^x$ terms to the Hamiltonian

Conclusion

- quantum annealer = universal analog quantum computer
  - specialized for optimization problems
  - exploited for quantum simulation
- quantum simulation
  1. equilibrium simulation
     - quantum annealers efficiently simulated with QMC methods
  2. closed-system dynamics
     - no known efficient generally aplicable classical algorithm
     - shorter quench times make this possible on quantum annealers
       $\rightarrow$ quantum advantage