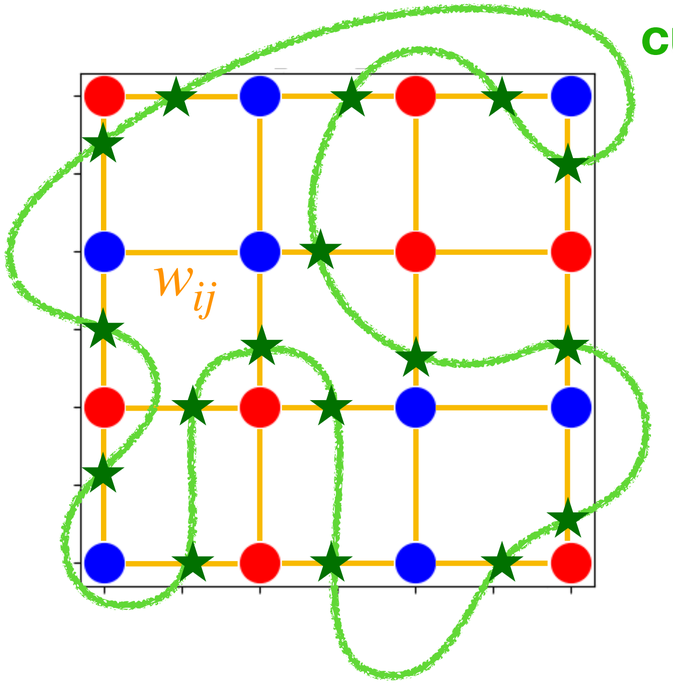
Max-Cut Project

Group Meeting - 08/14/2020

Max-Cut Problem & Antiferromagnetic Ising Model

Max-Cut Problem *(NP-hard)*



- Objective: Find cut that maximizes the total weight of edges in the cut: $\sum_{(ij)\in E(S,\bar{S})} w_{ij} d_{ij}$

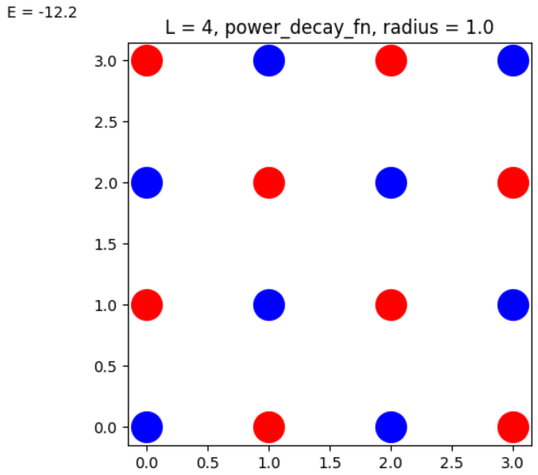
Antiferromagnetic Ising Model *(Mother nature!)*

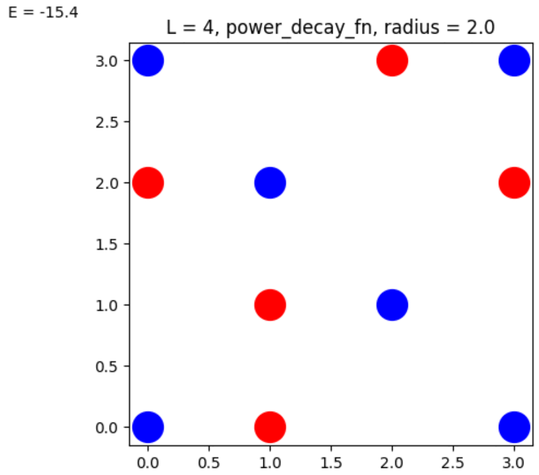
- Atoms i and interaction strengths $-J_{ij}$, $J_{ij} < 0$
- Anti-alignment:
  - spins σ_i^z: $(+1, -1)$
  - Interactions between anti-aligned spins: $\sigma_i^z \neq \sigma_j^z$

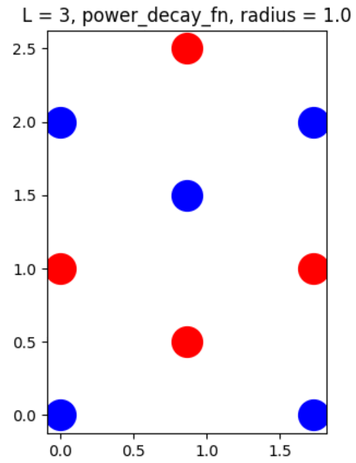
- Ground state: configuration that minimizes $H(\sigma) = -\sum_{ij} J_{ij}\sigma_i\sigma_j = -\sum_{ij} J_{ij} + 2\sum_{ij:\sigma_i\neq\sigma_j} J_{ij}$

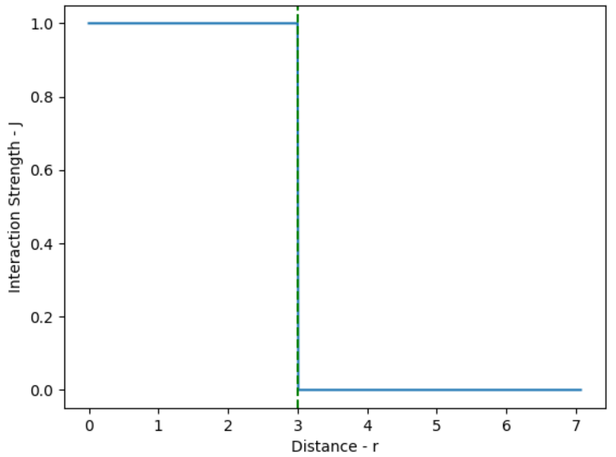
System Configurations

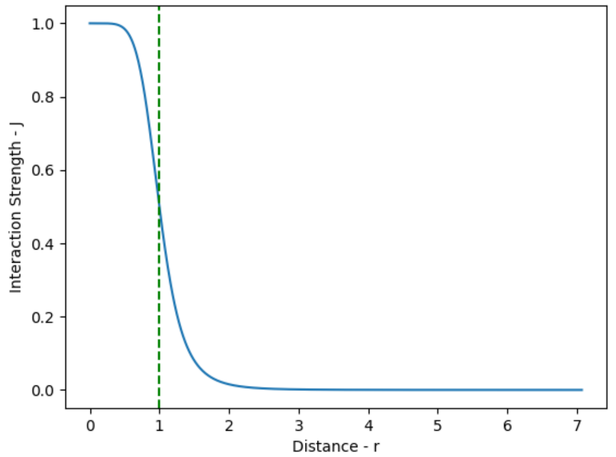
- **System structure**
  - Square lattice
  - Triangular lattice
  - Free particles
- **System size**
- **Interaction shape & range (radius, R)**
  - Step function $1 \cdot (d \leq R)$
  - Soft-core potential $\dfrac{1}{1+\left(\dfrac{d}{R}\right)^6}$
  - Random $R[0,1]$







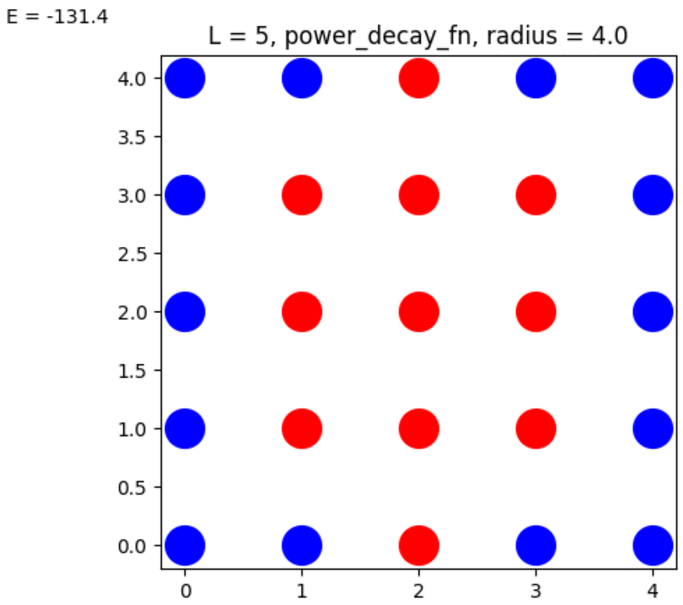




Classical Algorithms

Simulated Annealing

- Initialize a random partition (randomly assign each vertex to either set)
- Set initial temperature $T := T_0$
- Repeat t_{eq} iterations for equilibration ($t_{eq} = 1$ in continuous cooling):
  - Pick a random vertex v
  - $\Delta E =$ change of energy implied by switching the assignment of v: $p(v)$
  - If $R[0,1] < e^{-\Delta E/T}$ (using **Metropolis-Hastings Algorithm**):
    - $p(v) := -p(v)$
- Decrease temperature $T := r \cdot T$ (geometric cooling)
- Repeat steps 3 & 4 until convergence

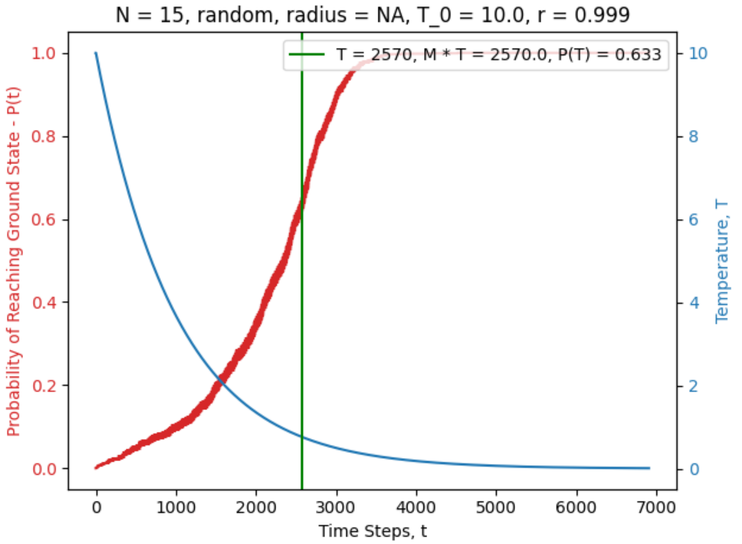


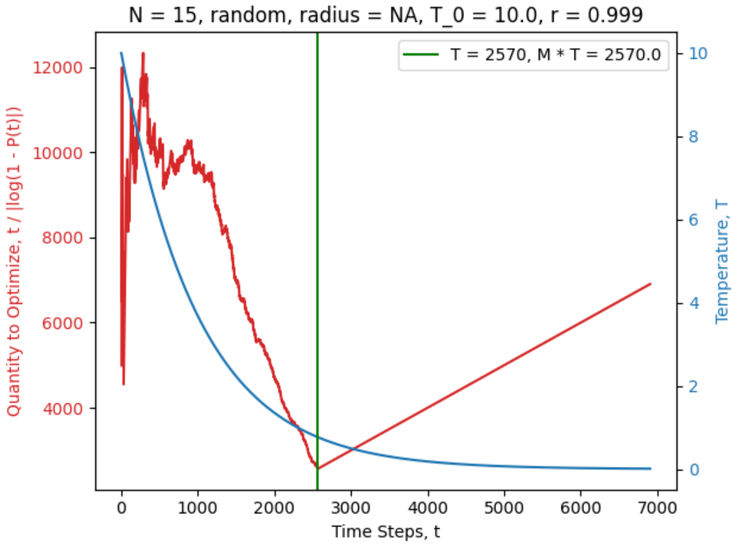
Algorithm Parameters:

- Initial temperature T_0
- Cooling rate r
- Equilibration duration t_{eq}

Algorithm Evaluation Metric

- Evaluation metric: **minimize** $M(T) \cdot T$
- In each run, $P(T)$ of finding the ground state estimated from N runs, where T is the # of steps
- $P_* = 1 - \varepsilon = 1 - \frac{1}{e}$
- Optimization parameters: M runs each for a time T
- Probability of not finding ground state: $(1 - P(T))^M = \varepsilon$
- $$M(T) = \begin{cases} \frac{\log \varepsilon}{\log(1 - P(T))} = \frac{\log(1 - P_*)}{\log(1 - P(T))}, & \text{if } P(T) < P_* \\ 1, & \text{if } P(T) \geq P_* \end{cases}$$
- Total # of steps: $$M(T) \cdot T \propto \begin{cases} \frac{T}{\log(1 - P(T))}, & \text{if } P(T) < P_* \\ T, & \text{if } P(T) \geq P_* \end{cases}$$

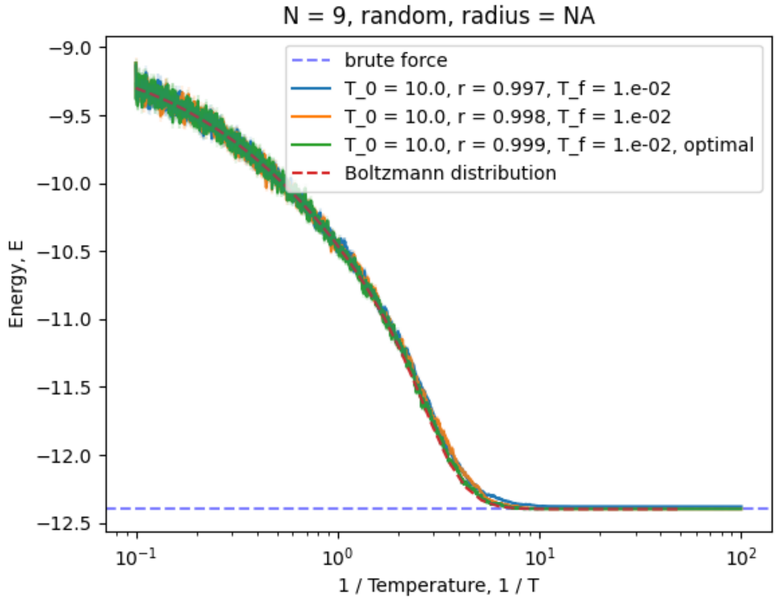


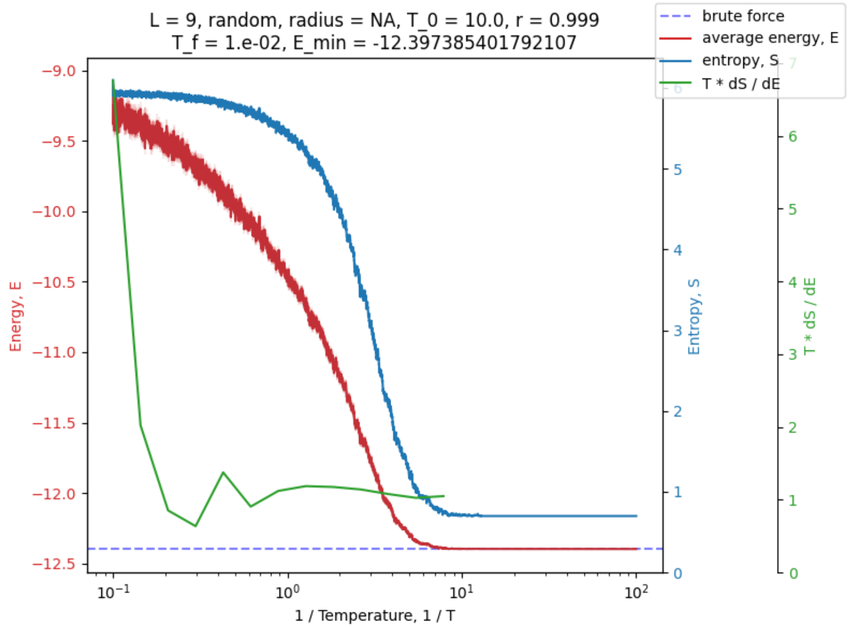


Sample Case:
All-to-all Random Interactions, N = 9

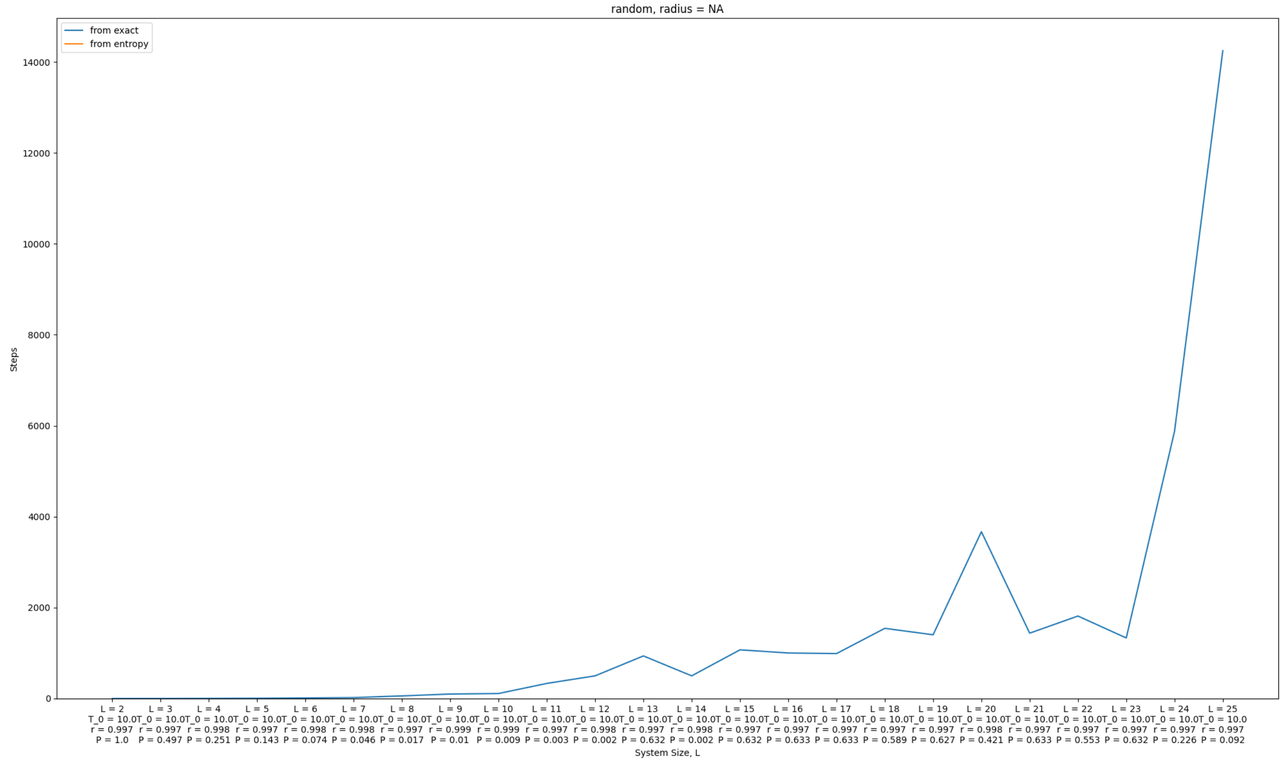
- Simulated Annealing (approximate)
  - Evaluation metric: minimize $M(T) \cdot T$
- Compare with: Brute Force Solution (exact)
  - Boltzmann distribution plotted using all states explored by brute force algorithm:

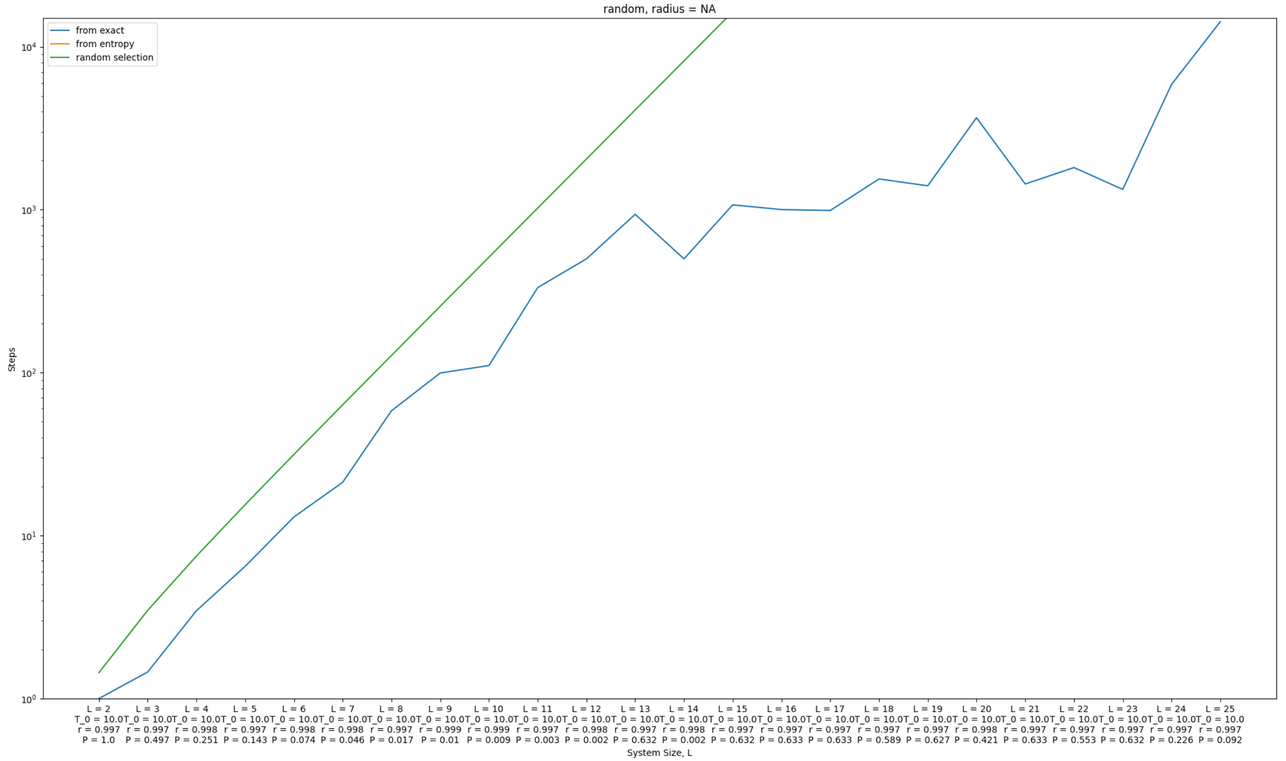
$$\frac{\sum_i E_i e^{-E_i/T}}{\sum_i e^{-E_i/T}}$$





Scaling with System Size





Quantum Algorithms

Adiabatic Quantum Evolution (AQE)

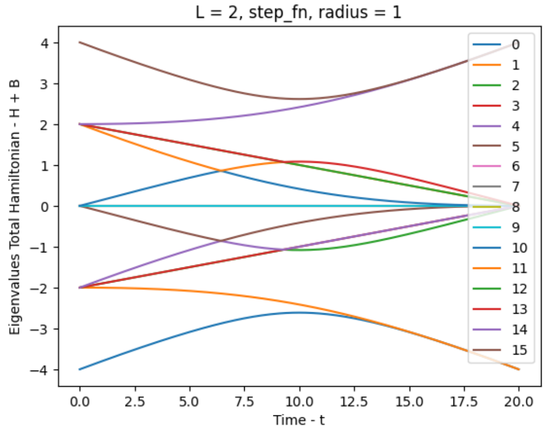
Ising Interaction Hamiltonian: $\hat{H}(\sigma) = -\sum_{ij} J_{ij}\sigma_i^z\sigma_j^z$, Reference Hamiltonian: $\hat{B}(\sigma) = -\sum_i \sigma_i^x$

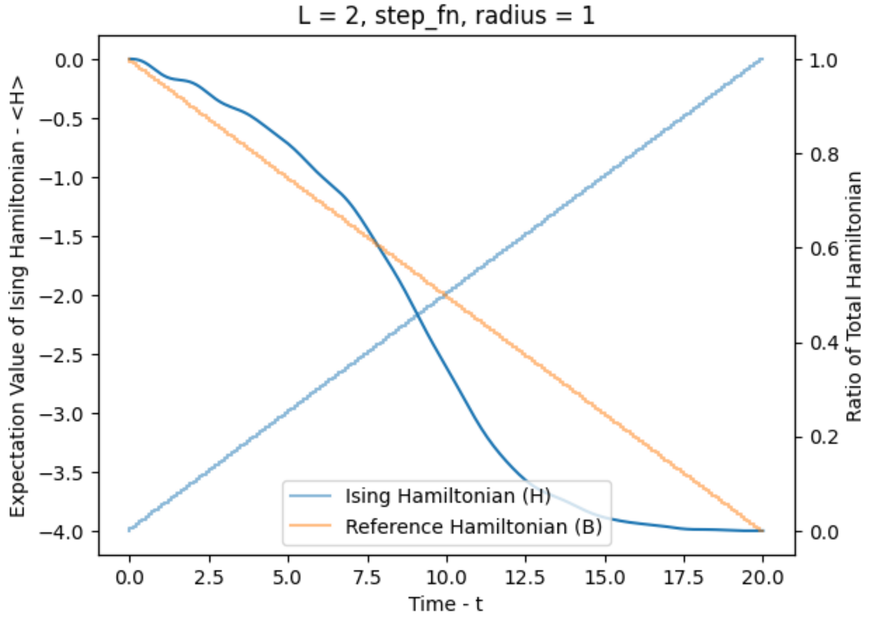
Evolution Hamiltonian: $\hat{H}(\tau) = (1-\tau)\hat{B} + \tau\hat{H}, \tau \in [0,1]$

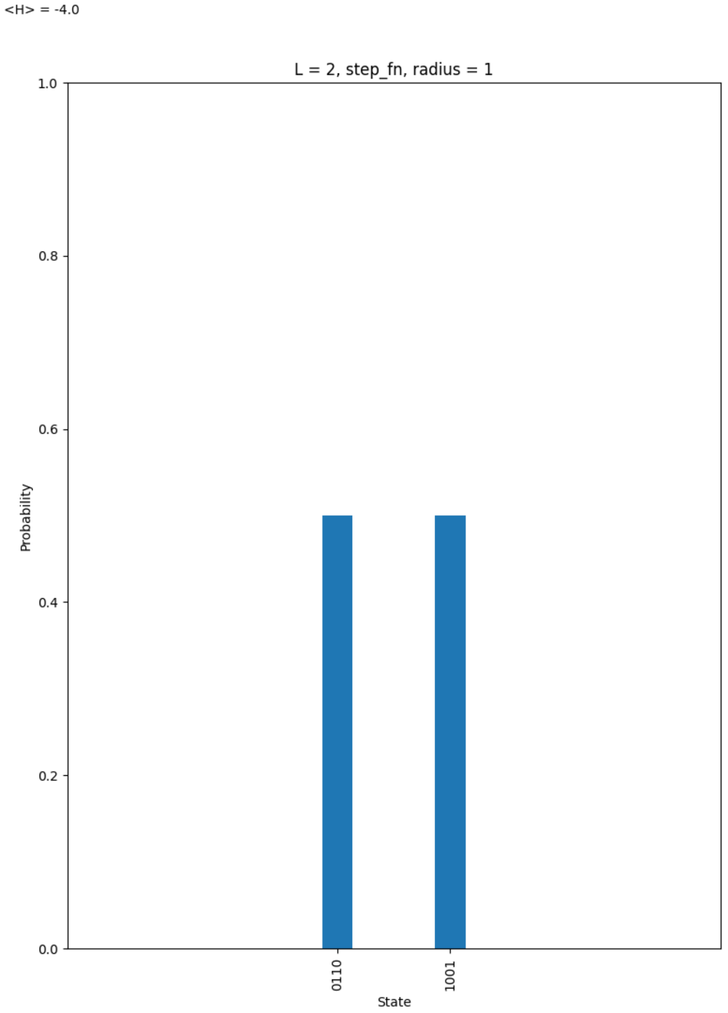
Initial state = ground state of $\hat{B}(\sigma)$: $\left|\psi_0\right\rangle = \left|+\right\rangle_{N-1} \otimes \ldots \otimes \left|+\right\rangle_0$

Final state: $\left|\psi_f\right\rangle = \left|\psi(\tau=1)\right\rangle$

Objective to minimize: $\left\langle\psi_f\right|\hat{H}\left|\psi_f\right\rangle$







Quantum Approximate Optimization Algorithm (QAOA)

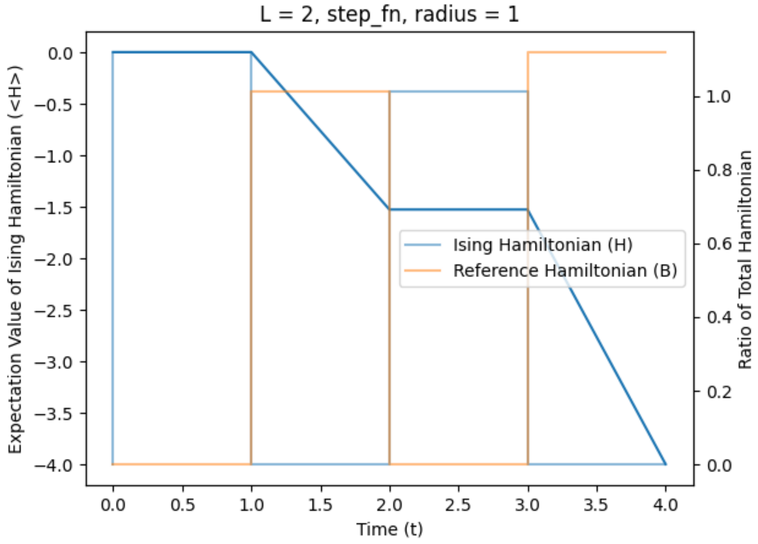
Ising Interaction Hamiltonian: $\hat{H}(\sigma) = -\sum_{ij} J_{ij}\sigma_i^z\sigma_j^z$, Reference Hamiltonian: $\hat{B}(\sigma) = -\sum_i \sigma_i^x$

Random initial state, e.g. ground state of $\hat{B}(\sigma)$: $\left|\psi_0\right\rangle = \left|+\right\rangle_{N-1} \otimes \ldots \otimes \left|+\right\rangle_0$

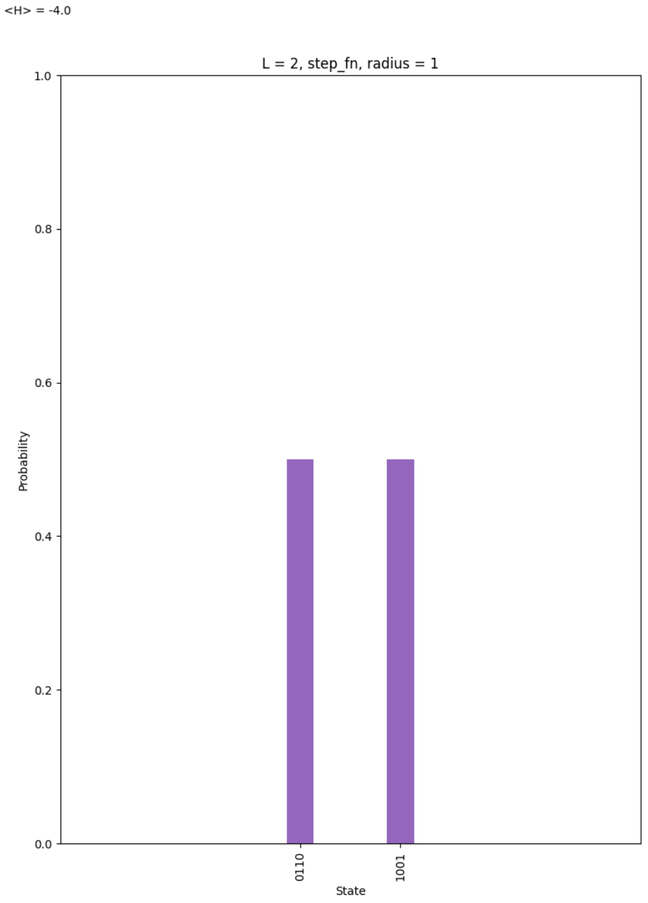
Unitary time evolution: $\hat{U}(\vec{\beta},\vec{\gamma}) = e^{-i\hat{B}\beta_{(\alpha-1)}}e^{-i\hat{H}\gamma_{(\alpha-1)}}\ldots e^{-i\hat{B}\beta_0}e^{-i\hat{H}\gamma_0}$

Final state: $\left|\psi_f(\vec{\beta},\vec{\gamma})\right\rangle = \hat{U}(\vec{\beta},\vec{\gamma})\left|\psi_0\right\rangle$

Objective to minimize: $\left\langle\psi_f(\vec{\beta},\vec{\gamma})\right|\hat{H}\left|\psi_f(\vec{\beta},\vec{\gamma})\right\rangle$



Optimization: $\vec{\beta},\vec{\gamma} = \text{VQE}\left(\text{ansatz} = \left|\psi_f(\vec{\beta},\vec{\gamma})\right\rangle, \text{operator} = \hat{H}\right)$



Algorithm Parameters:

- Circuit depth α
- Angles $\vec{\beta},\vec{\gamma}$

Optimization Method: Variational Quantum Eigensolver (VQE)

VQE $\left(\text{ansatz} = \left|\psi_f(\vec{\theta})\right\rangle, \text{operator} = \hat{H}\right)$:

== Classical optimization ==

- Initialize random parameters: $\vec{\theta} := \vec{\theta_0}$
- Loop until convergence:

  == Quantum sub-routine ===

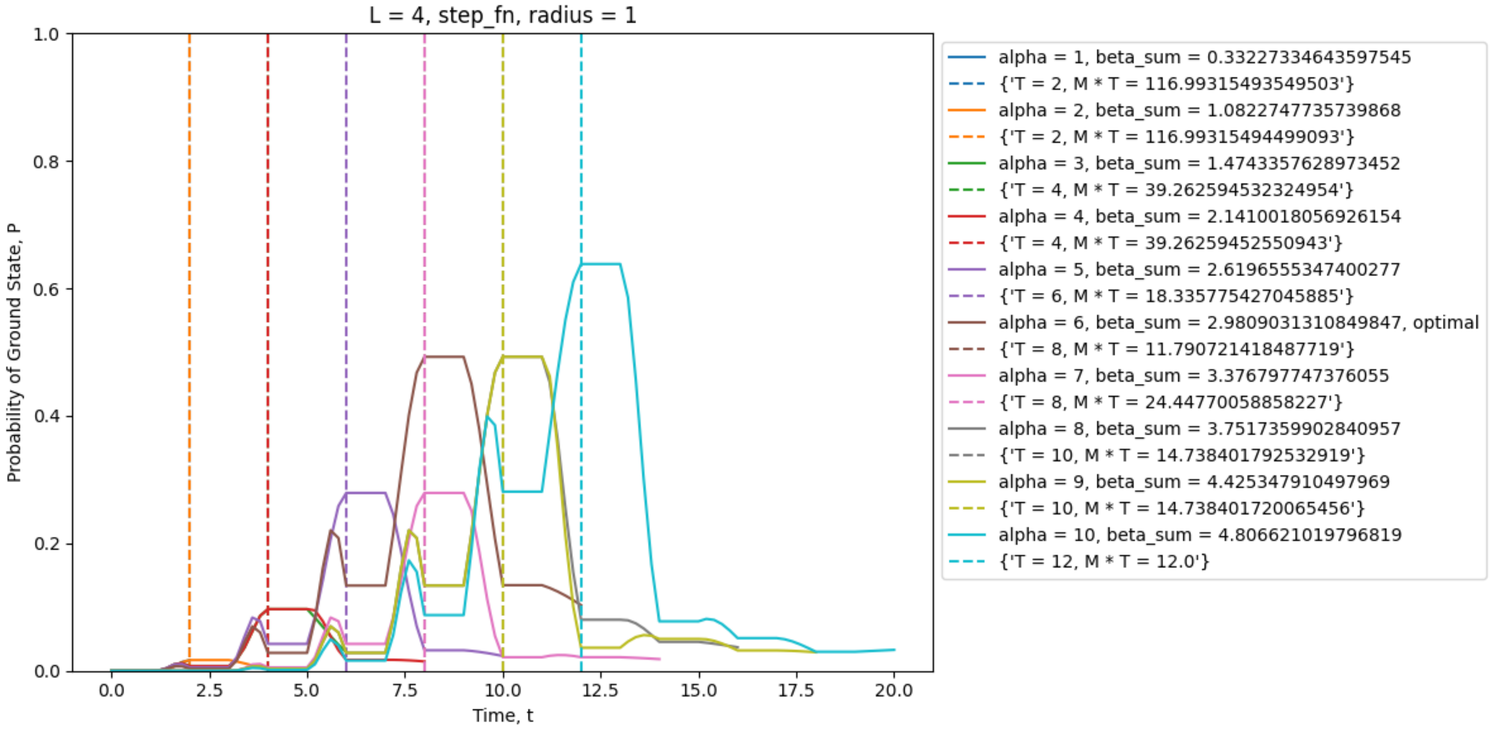
  - Prepare ansatz: $\left|\psi_f(\vec{\theta})\right\rangle$
  - Evaluate objective (expectation value of operator): $\left\langle \psi_f(\vec{\theta}) \middle| \hat{H} \middle| \psi_f(\vec{\theta}) \right\rangle$

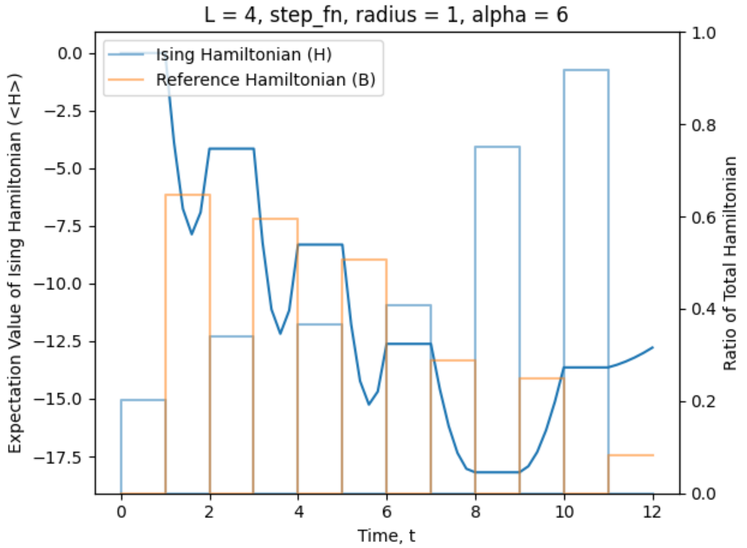
    $M(T) \cdot T$, where $T \in [1,\ 2\alpha]$
  - Update parameter $\vec{\theta}$:= optimizationStep($\vec{\theta}$)
  - Return parameters that minimize objective: $\vec{\theta} = \min\left(\left\langle \psi_f(\vec{\theta}) \middle| \hat{H} \middle| \psi_f(\vec{\theta}) \right\rangle\right)$

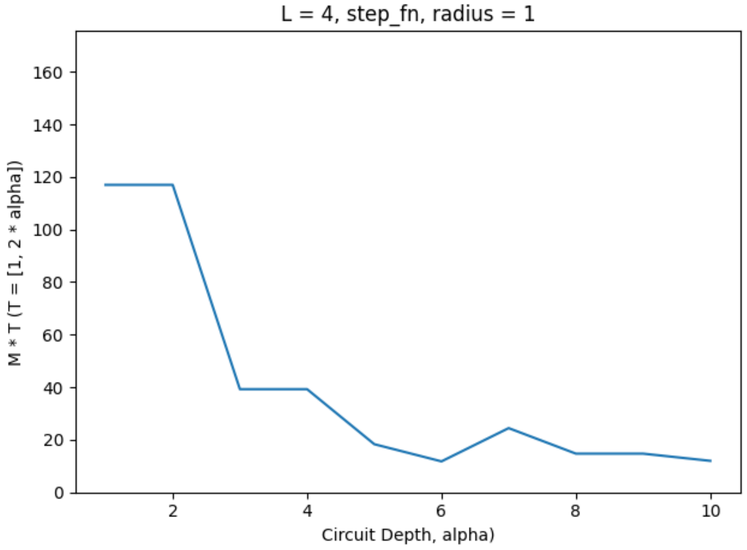
    $M(T) \cdot T$

Sample Case:
Nearest-Neighbor Interactions, Square Lattice, N = 4x4

- Variational Quantum Eigensolver (approximate)
  - Evaluation metric: minimize $M(T) \cdot T$, where $T \in [1,\ 2\alpha]$
- Quantum Approximate Optimization Algorithm (approximate)







Next Steps

- **Comparing classical & quantum algorithms**
  - Common optimization: minimize $M(T) \cdot T$, i.e. number of trials x number of “steps” per trial
  - No obvious one-to-one correspondence of the grounds for comparison: what is T?
    - Classical algorithm:
      - number of iterations of Simulated Annealing
    - Quantum algorithm:
      - Length of Hamiltonian pulse sequence, $[1,\ 2\alpha]$
      - Integrated interaction strength x time ($\sum_{i=0}^{\alpha-1} \beta_i$)
- **Classical & quantum speedups**
  - Different cooling schedules for Simulated Annealing
  - Different angle initializations for QAOA
- **Scaling to larger system sizes with reasonable simulation runtimes**
  - Entropy as heuristic for probability of reaching ground state in Simulated Annealing
  - DTWA for simulating larger quantum systems

Bibliography

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- http://www.mit.edu/~ilkery/papers/MetropolisHastingsSampling.pdf
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- https://journals.aps.org/prx/pdf/10.1103/PhysRevX.10.021067

- physical time for re-initializing the system when computing M * T, include overhead
- Integrated interaction strength is good because H is costly due to decay, include in simulation, in reality probability doesn’t strictly increase, T might be the argument at that maximum