Max-Cut Project

Rydberg Lab Meeting Update - 07/29/2020

Recap: Max-Cut Problem & Antiferromagnetic Ising Model

Max-Cut Problem

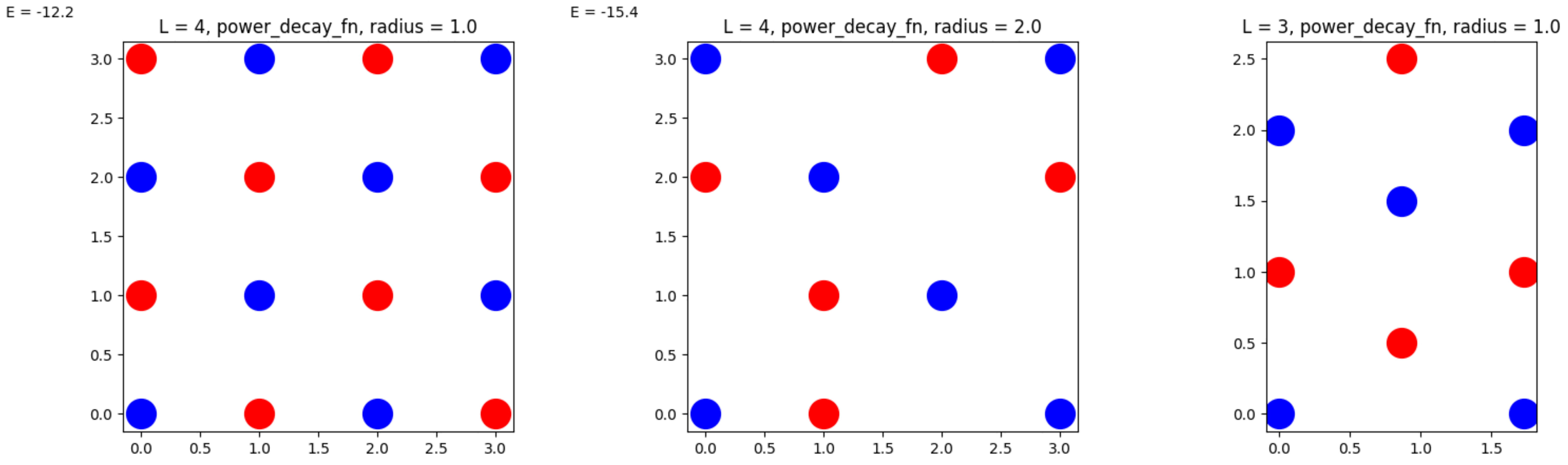
- Undirected graph: $G = (V, E)$
- Cut:
  - Partition: $(S \subseteq V, \bar{S} = V \backslash S)$
  - Set of edges with one vertex in S and one vertex in $\bar{S}$: $E(S, \bar{S})$
- Objective: Find cut that maximizes the total weight of edges in the cut: $\sum_{(ij) \in E(S,\bar{S})} w_{ij} d_{ij}$
- NP-hard

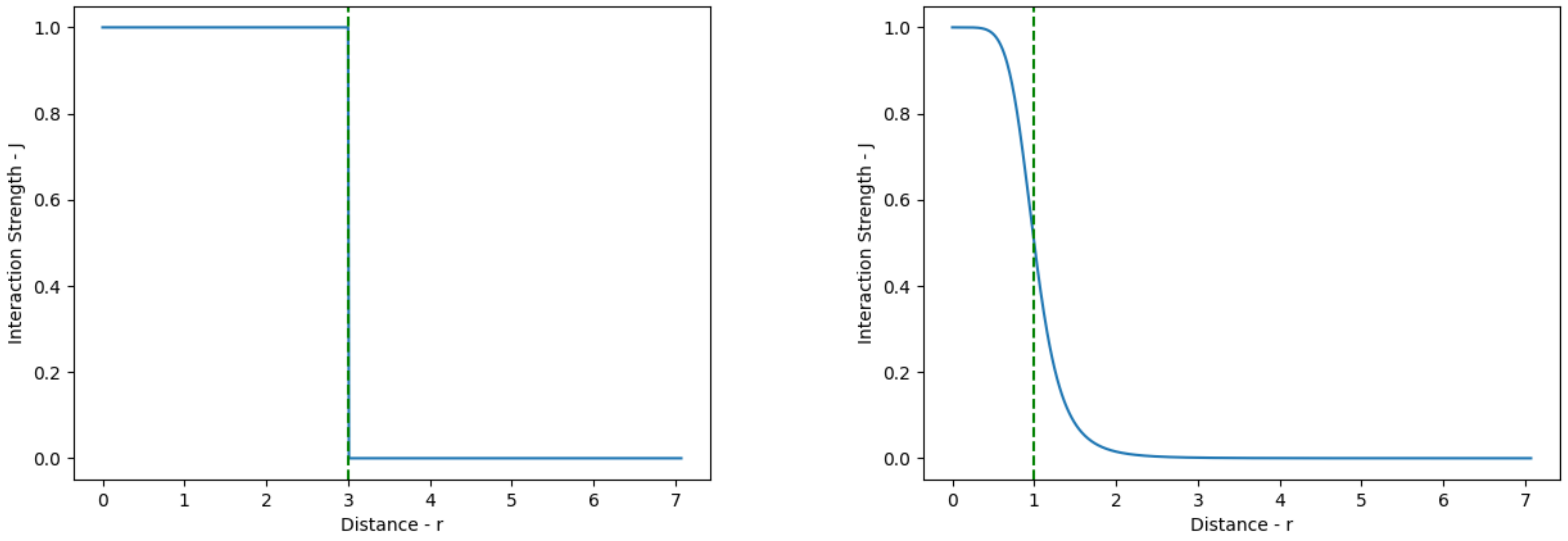
Antiferromagnetic Ising Model

- 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 $H(\sigma) = -\sum_{ij} J_{ij} \sigma_i \sigma_j = -\sum_{ij} J_{ij} + 2 \sum_{ij:\sigma_i \neq \sigma_j} J_{ij}$
- Mother nature!

System Configurations

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

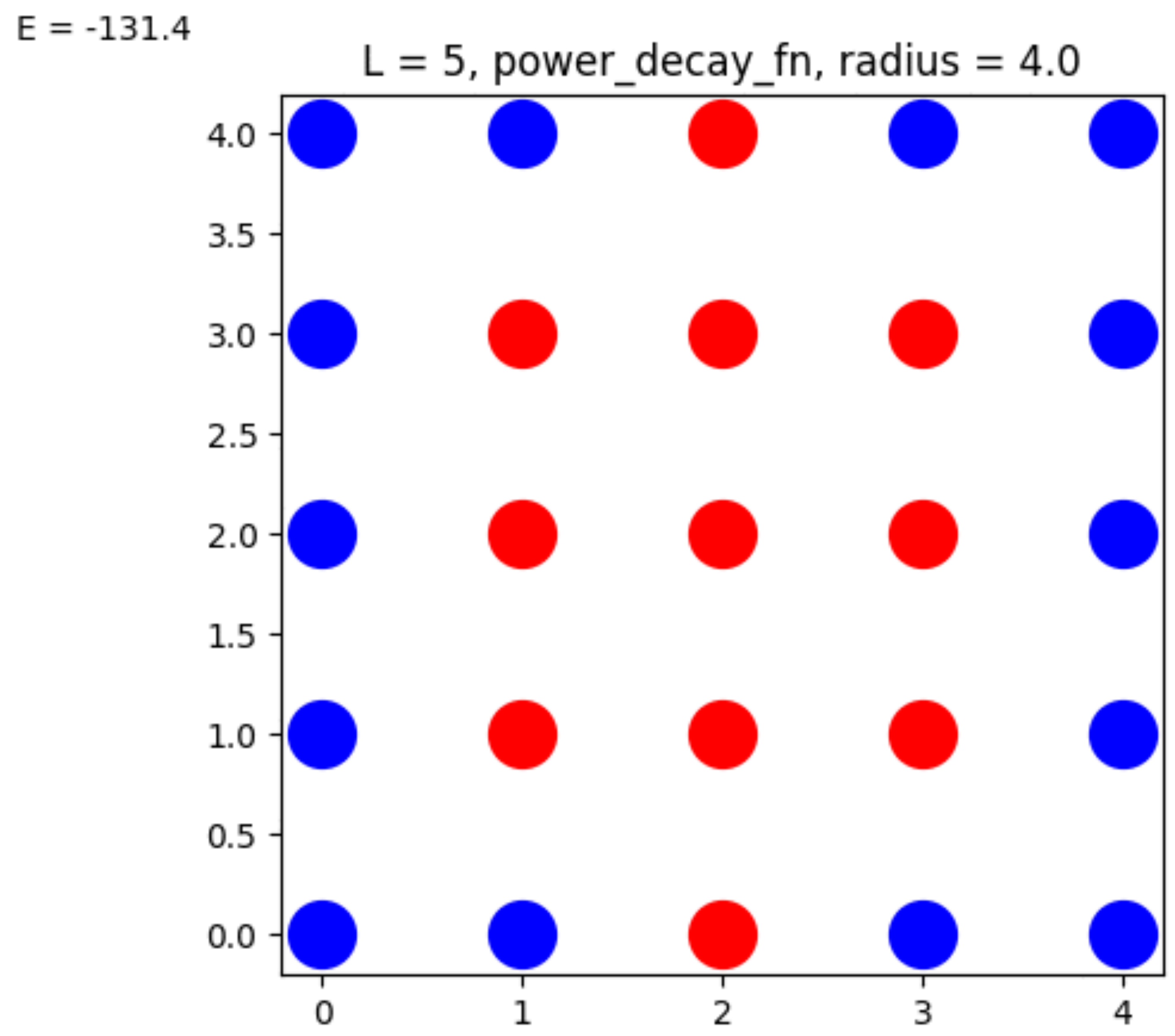




Classical Algorithms

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



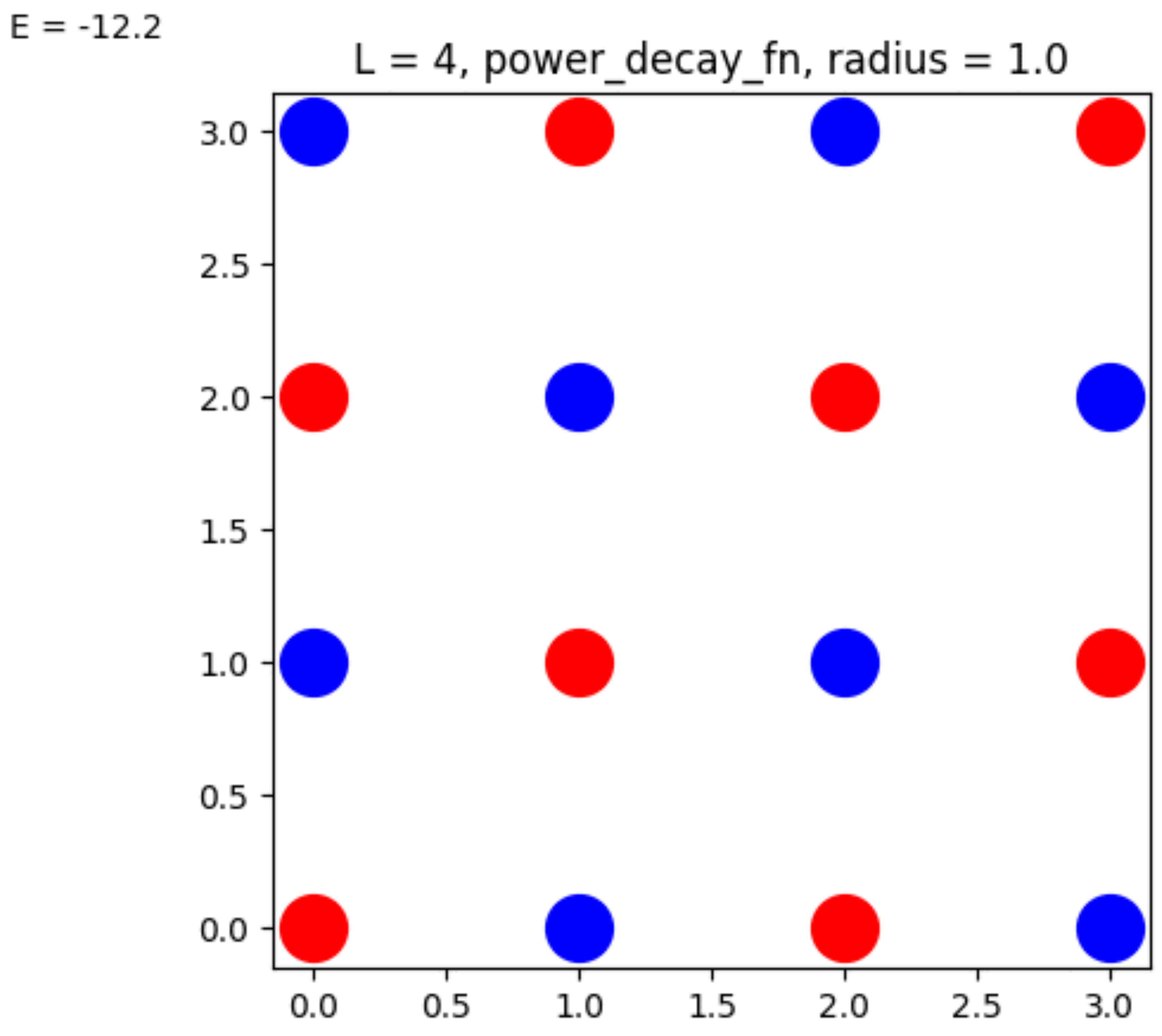
Algorithm Parameters:

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

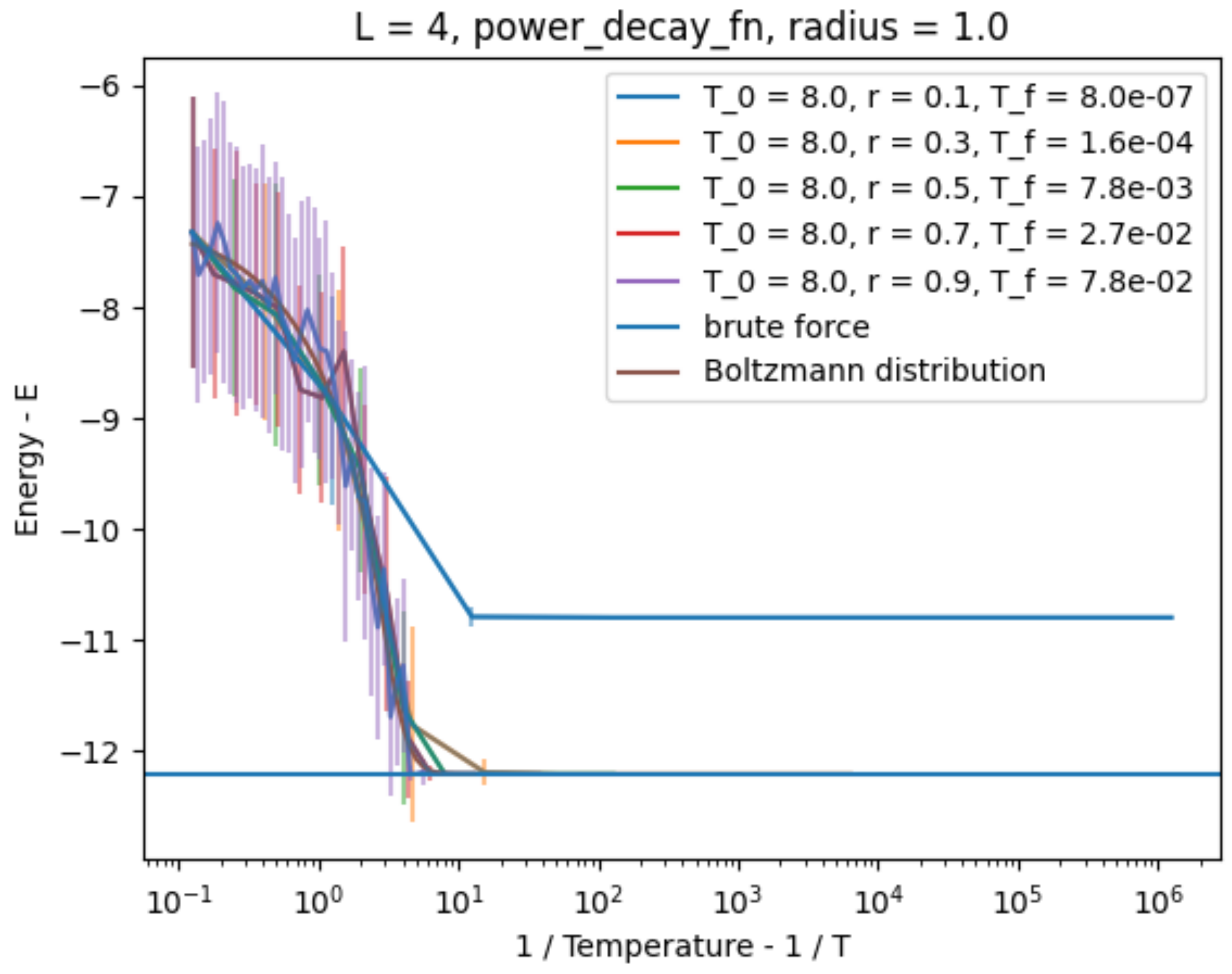
Sample Case: Square Lattice, Power Decay Function with $R = 1, t_{eq} = 1000$

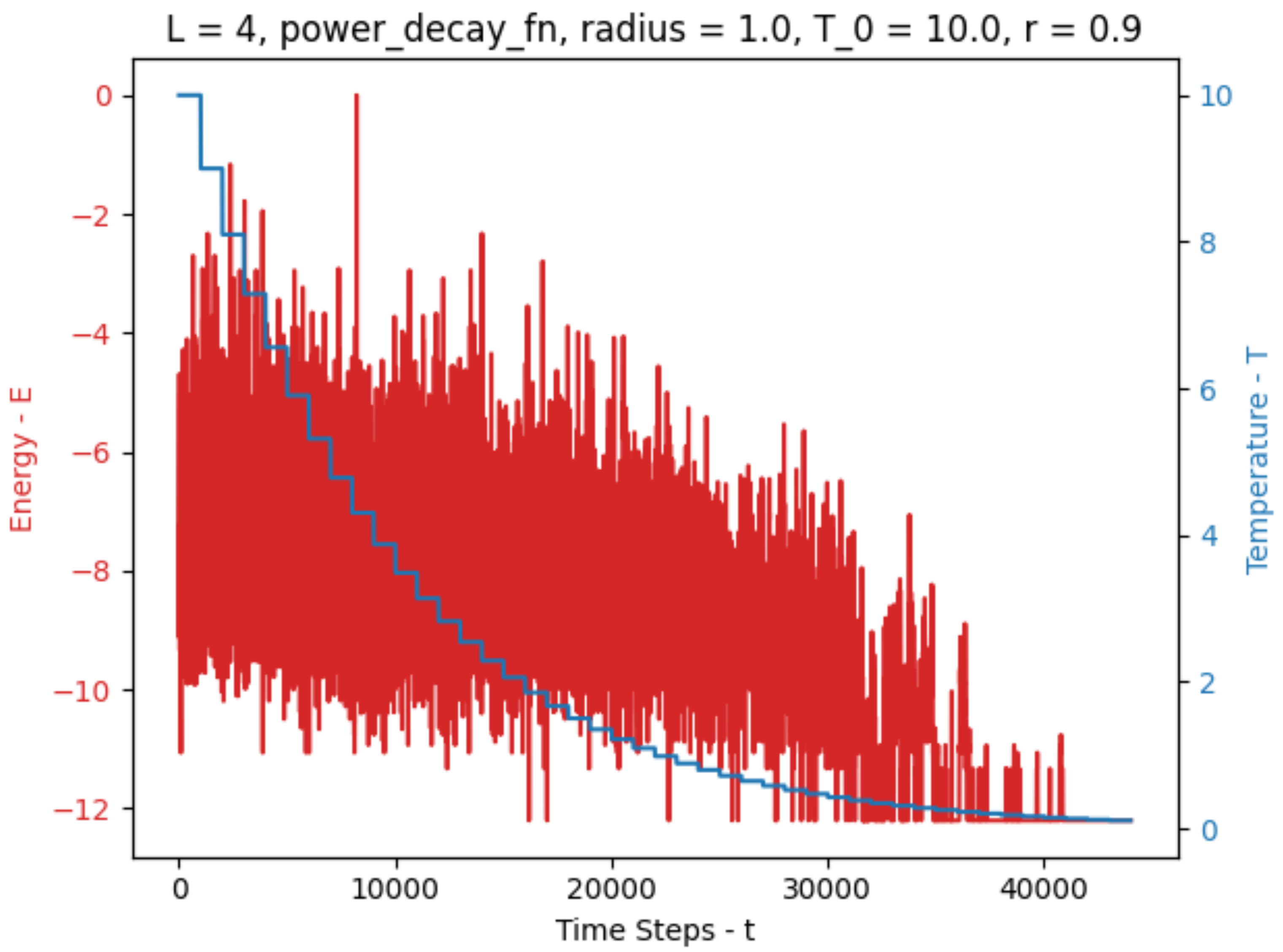
- Simulated Annealing (approximate)
  - Evaluation metric: reaching the minimum energy possible in the fastest number of steps averaged over 50 runs
- Compare with: Brute Force Solution (exact)
  - Boltzmann distribution plotted using all states explored by brute force algorithm:

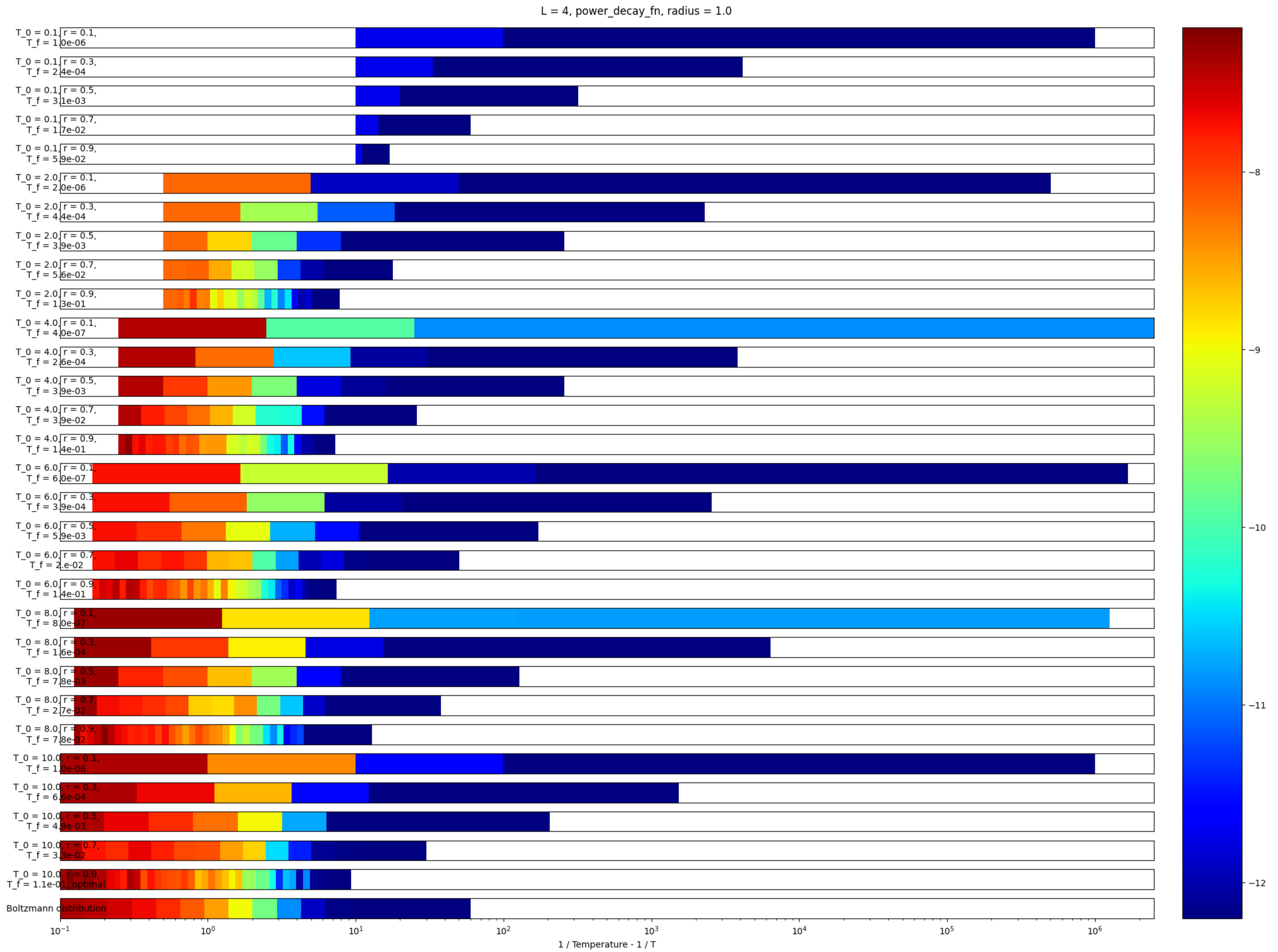
$$\frac{\sum_i E_i e^{-E_i/T}}{\sum_i e^{-E_i/T}}$$



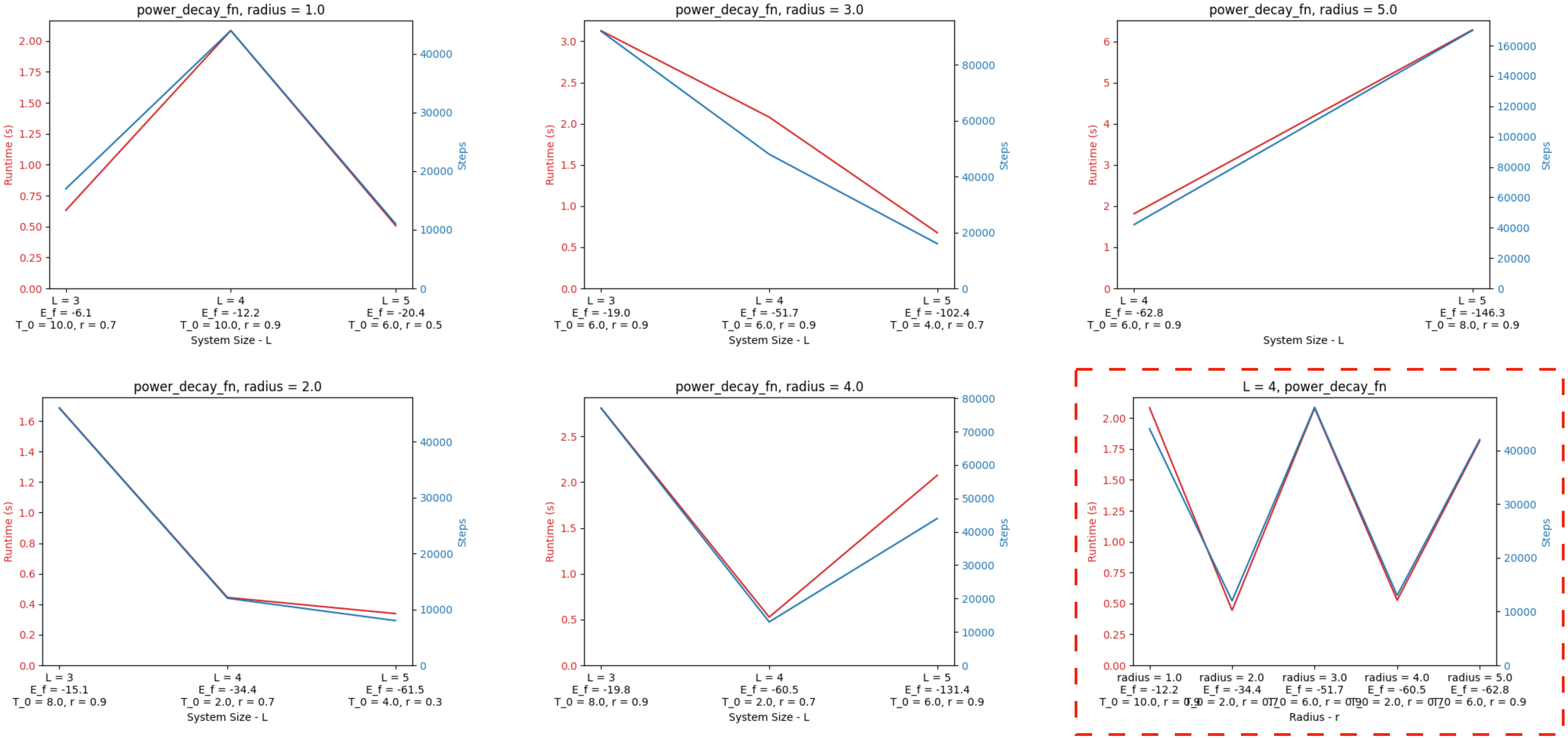
Algorithm Parameter Optimization







Results: Scaling with Radius, System Size

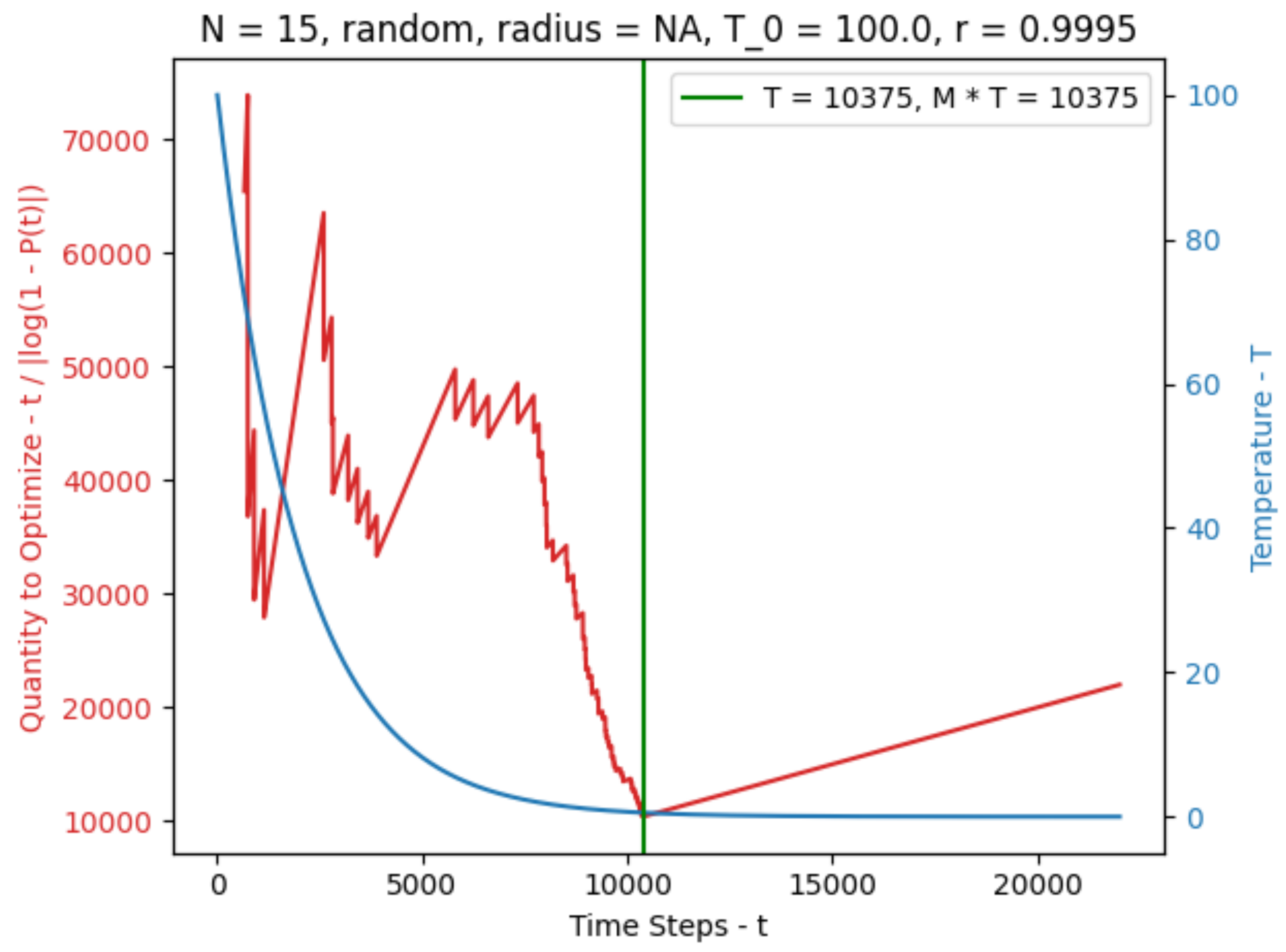


Current Focus:

Random interactions, Free particles, $t_{eq} = 1$ (continuous cooling)

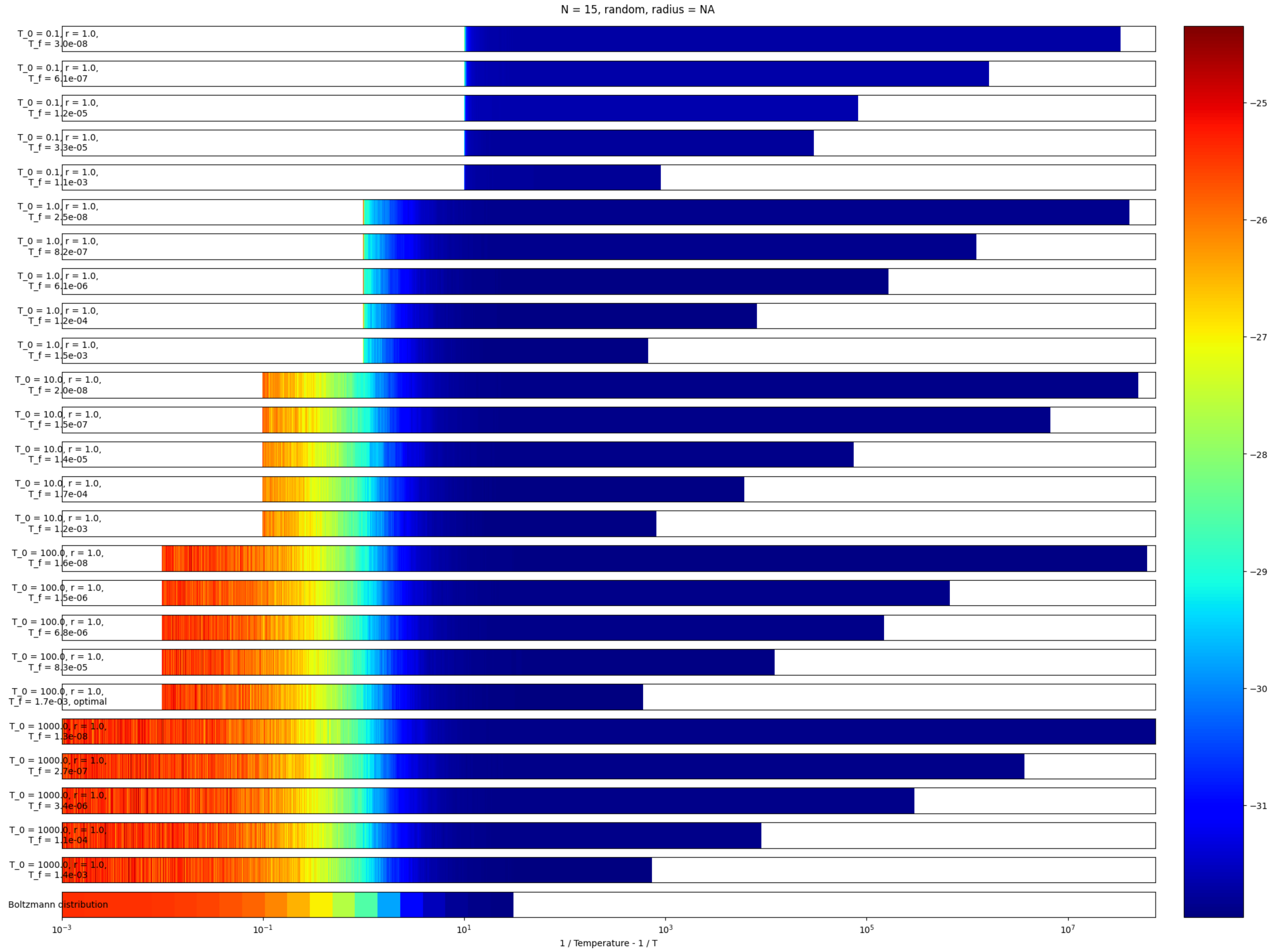
- Goal: observe exponential scaling with system size
- Simulated Annealing (approximate)
  - New evaluation metric: minimize $M(T) \cdot T$
- Compare with: Brute Force Solution (exact)
  - Boltzmann distribution plotted using all states explored by brute force algorithm:

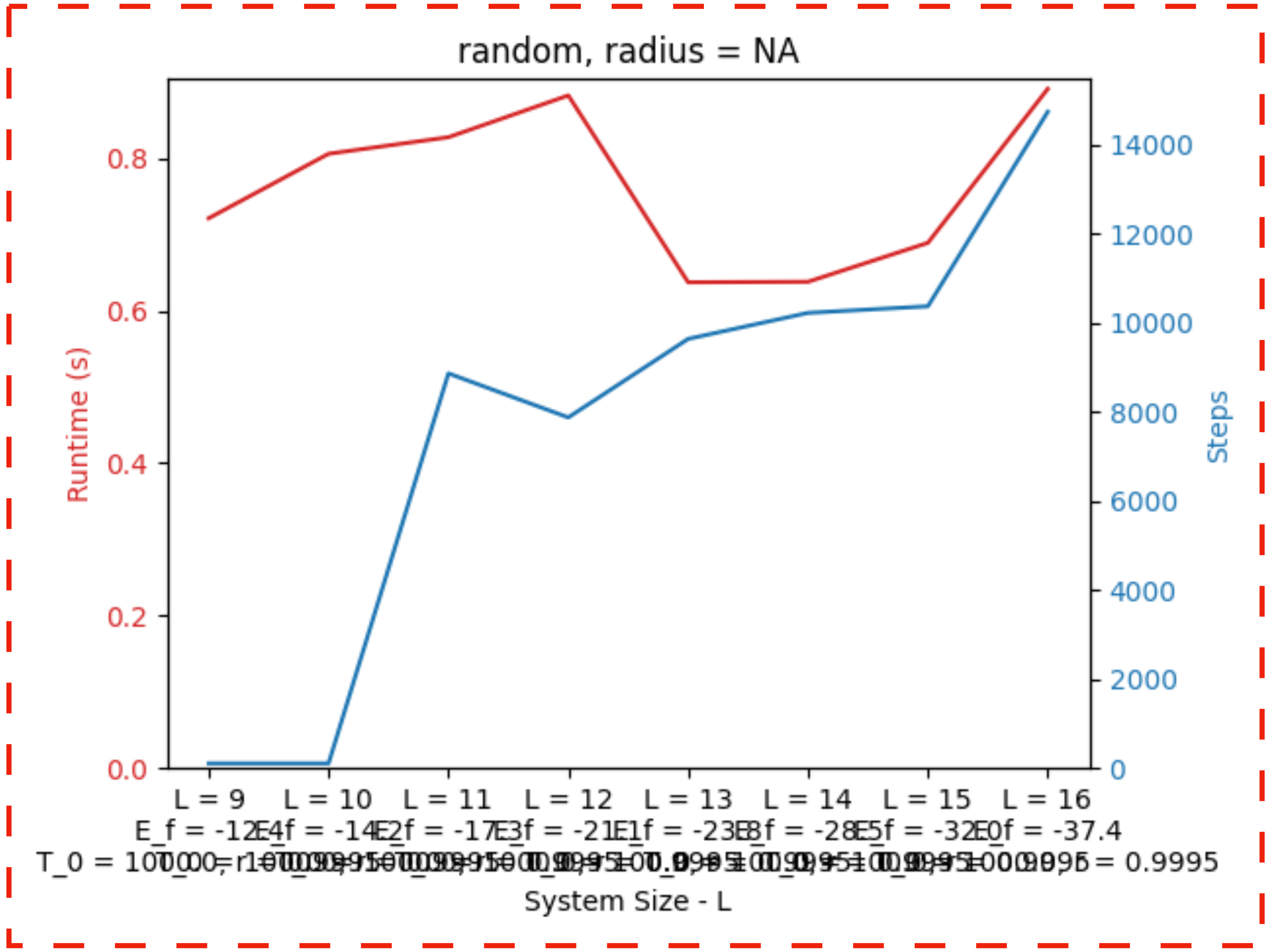
$$\frac{\sum_i E_i e^{-E_i/T}}{\sum_i e^{-E_i/T}}$$

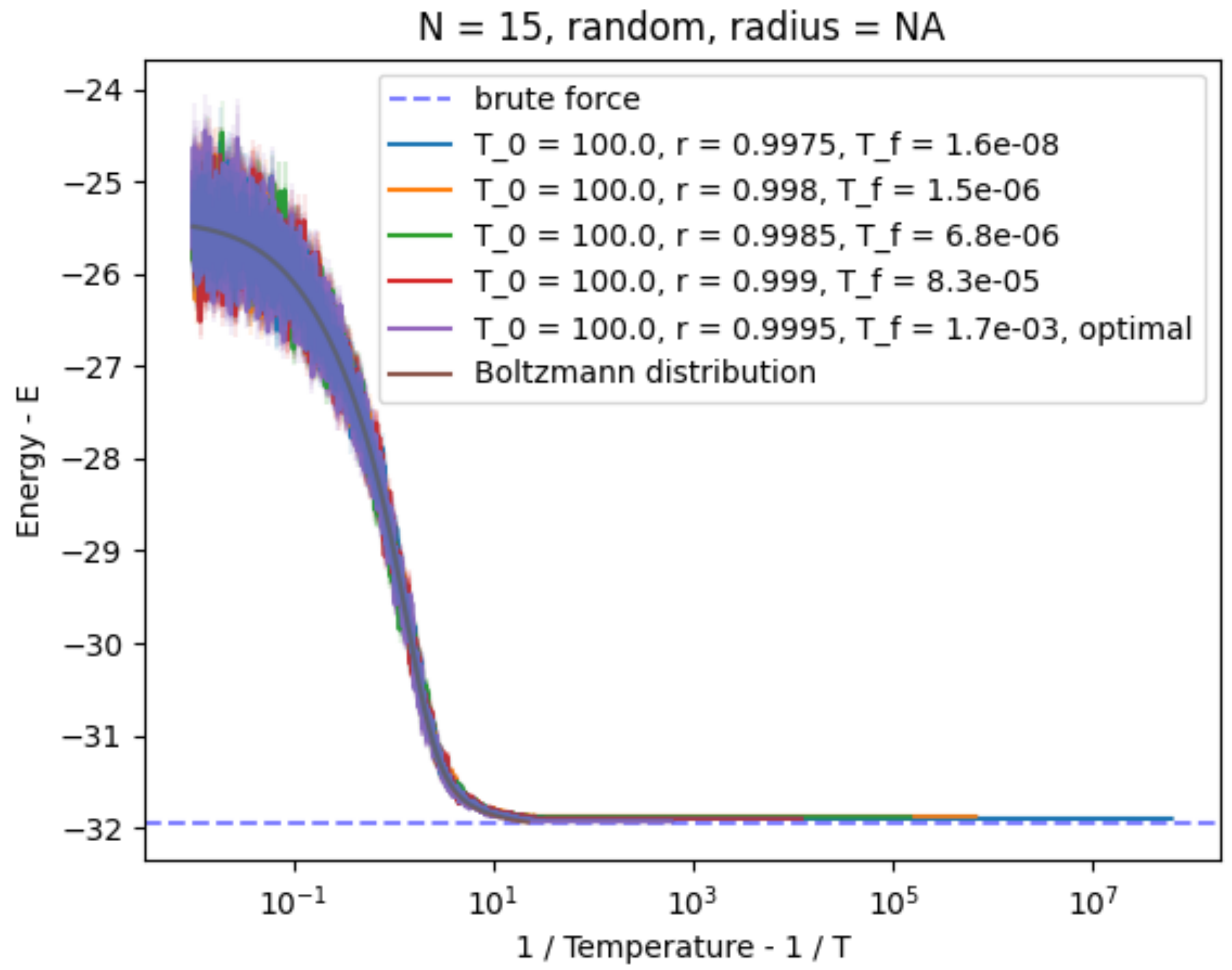


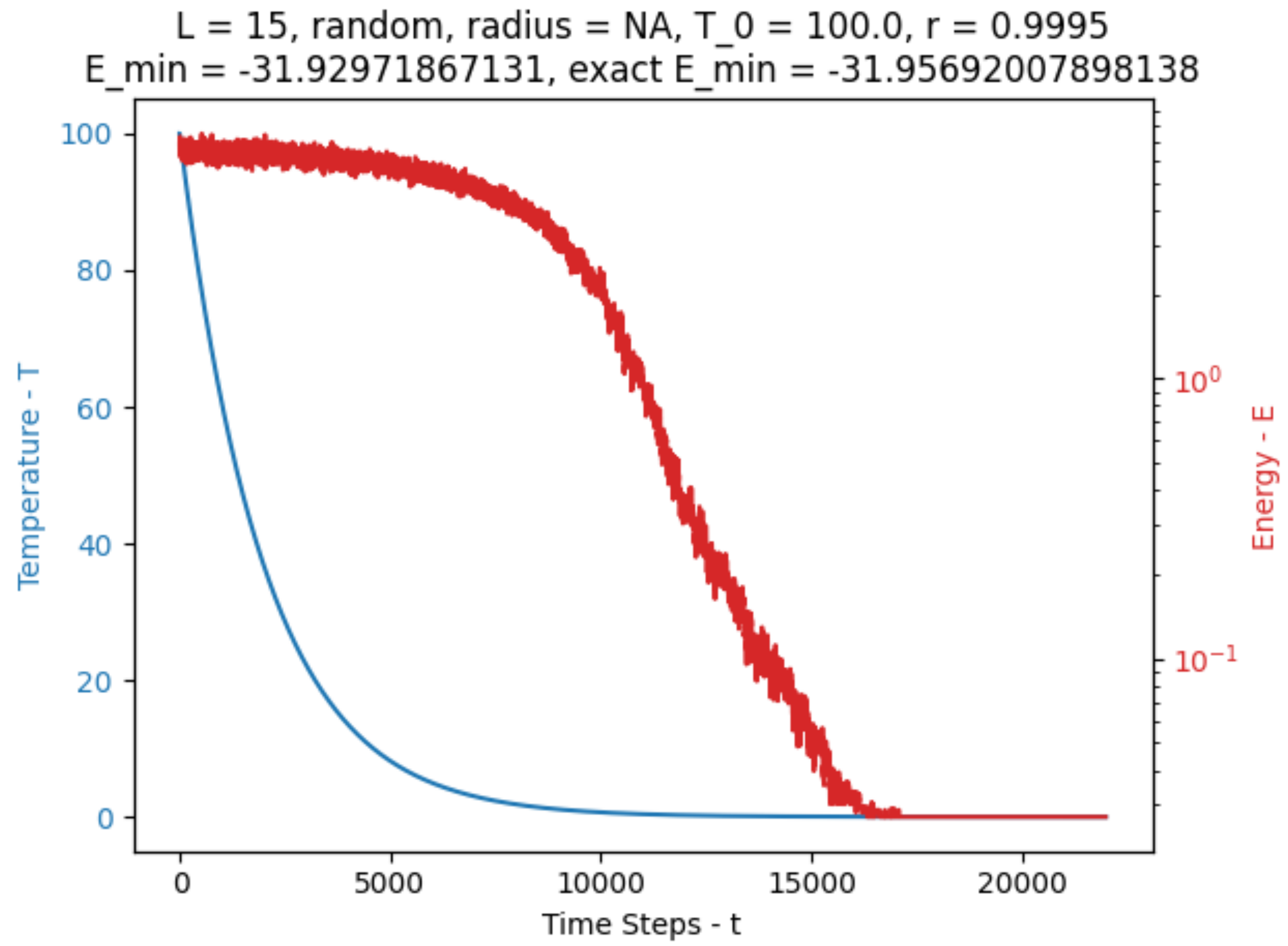
- In each run, $P(T)$ of finding the ground state estimated from N runs, where T is the # of steps
- $P_* = 1 - \varepsilon = 1 - \dfrac{1}{e}$
- Optimization parameters: M runs each for a time T
- Probability of not finding ground state: $(1 - P(T))^M = \varepsilon$
- $$M(T) = \begin{cases} \dfrac{\log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

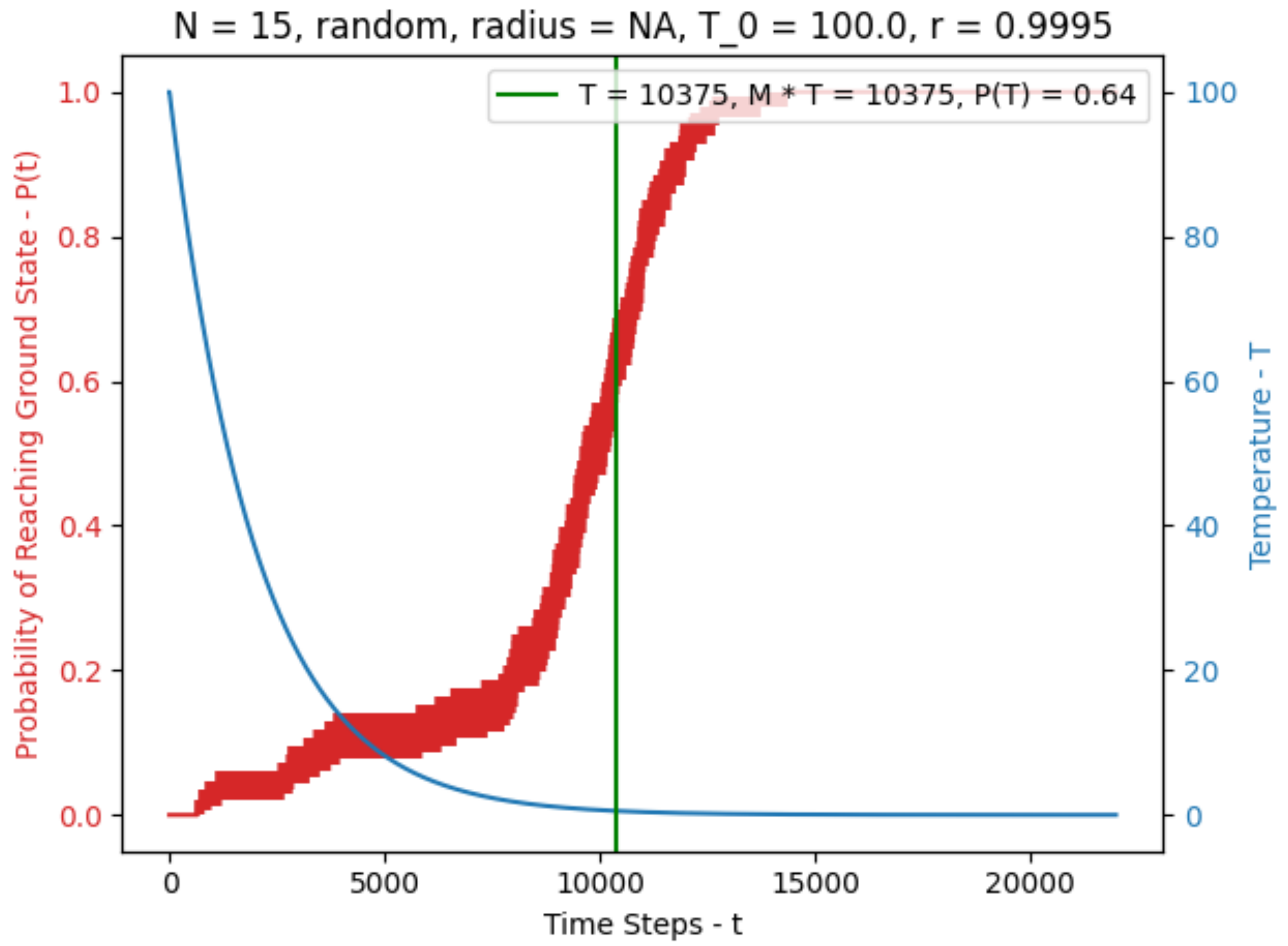
$$M(T) \cdot T \propto \begin{cases} \dfrac{T}{\log(1-P(T))}, & \text{if } P(T) < P_* \\ T, & \text{if } P(T) \geq P_* \end{cases}$$


N = 15, random, radius = NA
Boltzmann distribution
1 / Temperature - 1 / T


random, radius = NA
Runtime (s)
Steps
L = 9
L = 10
L = 11
L = 12
L = 13
L = 14
L = 15
L = 16
System Size - L


N = 15, random, radius = NA
brute force
T_0 = 100.0, r = 0.9975, T_f = 1.6e-08
T_0 = 100.0, r = 0.998, T_f = 1.5e-06
T_0 = 100.0, r = 0.9985, T_f = 6.8e-06
T_0 = 100.0, r = 0.999, T_f = 8.3e-05
T_0 = 100.0, r = 0.9995, T_f = 1.7e-03, optimal
Boltzmann distribution
Energy - E
1 / Temperature - 1 / T


L = 15, random, radius = NA, T_0 = 100.0, r = 0.9995
E_min = -31.92971867131, exact E_min = -31.95692007898138
Temperature - T
Energy - E
Time Steps - t


N = 15, random, radius = NA, T_0 = 100.0, r = 0.9995
T = 10375, M * T = 10375, P(T) = 0.64
Probability of Reaching Ground State - P(t)
Temperature - T
Time Steps - t

Next Steps

- Random interactions between free particles
    - Scale out to larger systems to hopefully observe exponential growth in complexity
    - Evaluation metric for larger systems (where brute force solutions are not feasible): entropy ($E[-\log P]$) across different runs
- Distance-dependent interactions between particles organized as square/isometric lattice
    - We'll see once we have the exponential scaling in the random case!

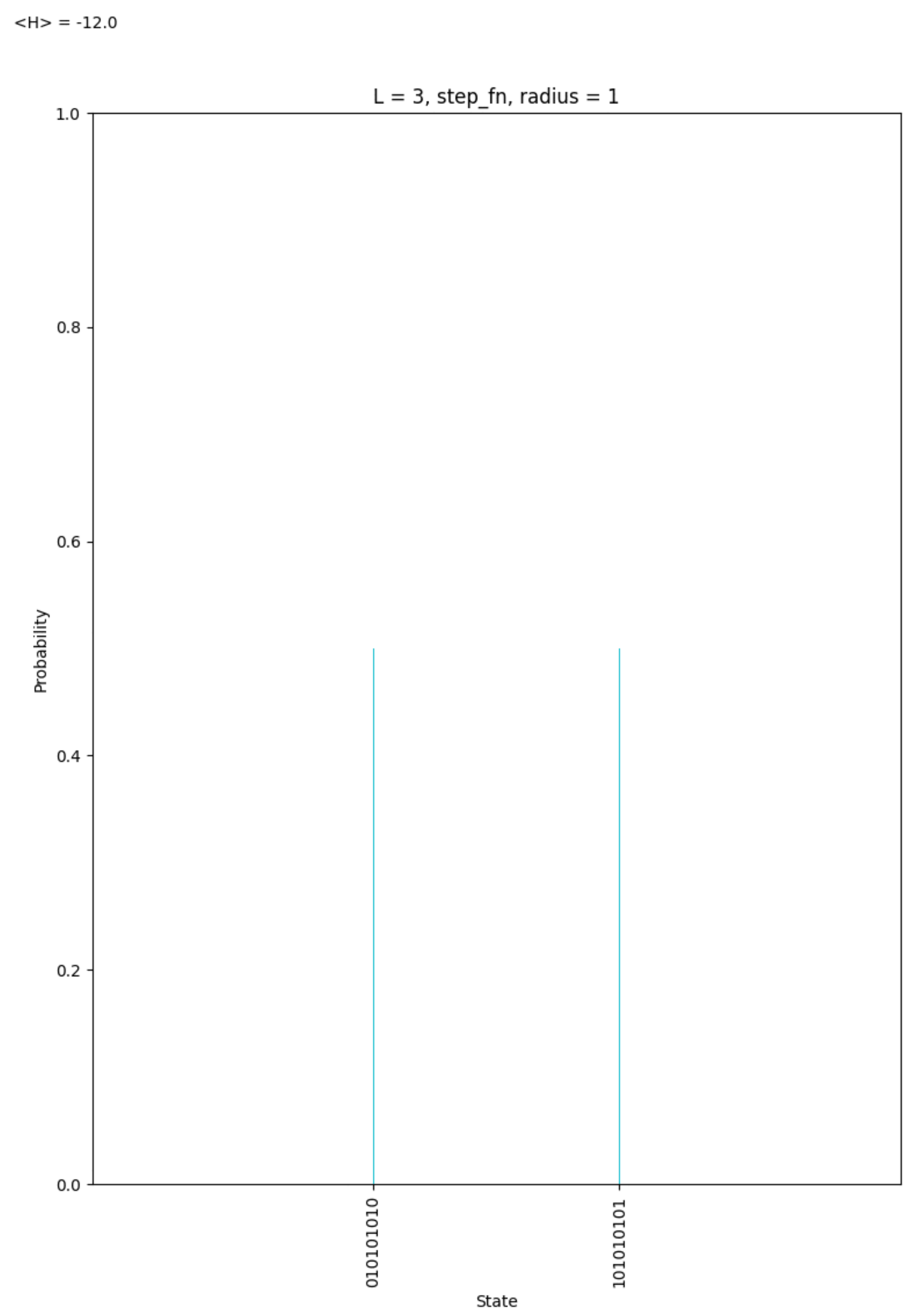
Quantum Algorithms

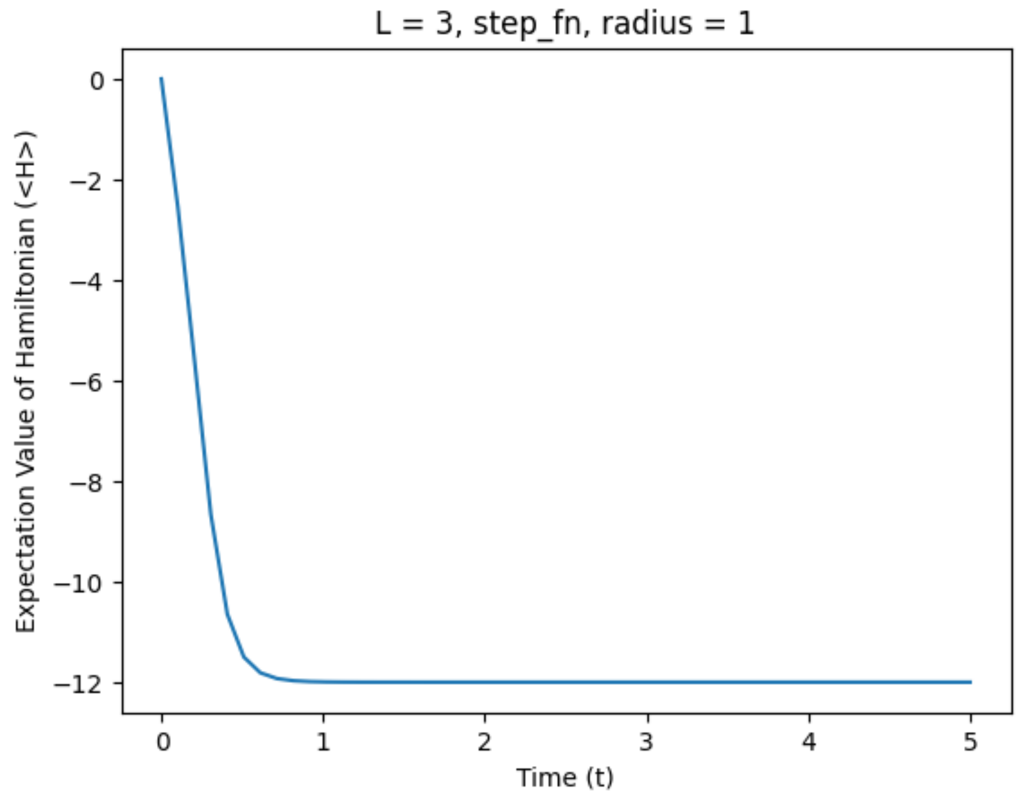
Benchmarking: QuSpin vs. NumPy/SciPy/TamLib

Metric: Runtime of imaginary time evolution, which finds the ground states of a Hamiltonian by making the substitution $t \to i\tau$ in the corresponding unitary time evolution $\left|\psi(\tau)\right\rangle = e^{i\hat{H}t}\left|\psi(0)\right\rangle = e^{-\hat{H}\tau}\left|\psi(0)\right\rangle = \sum_i e^{-\hat{E}_i\tau}\left|\psi_i(0)\right\rangle$.

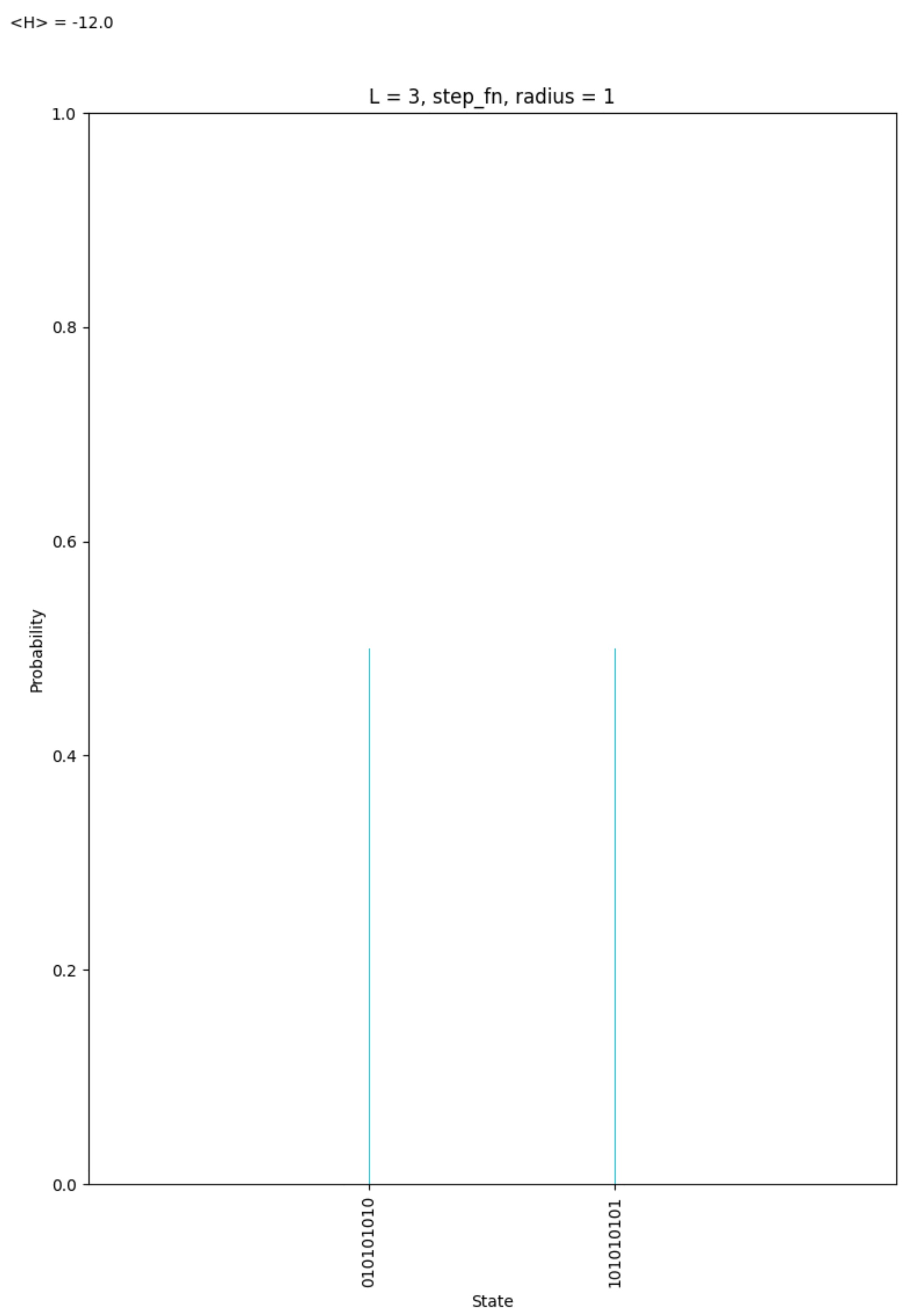
At $\tau \to \infty$, all terms except for the state with minimum energy decay, resulting in the ground state.

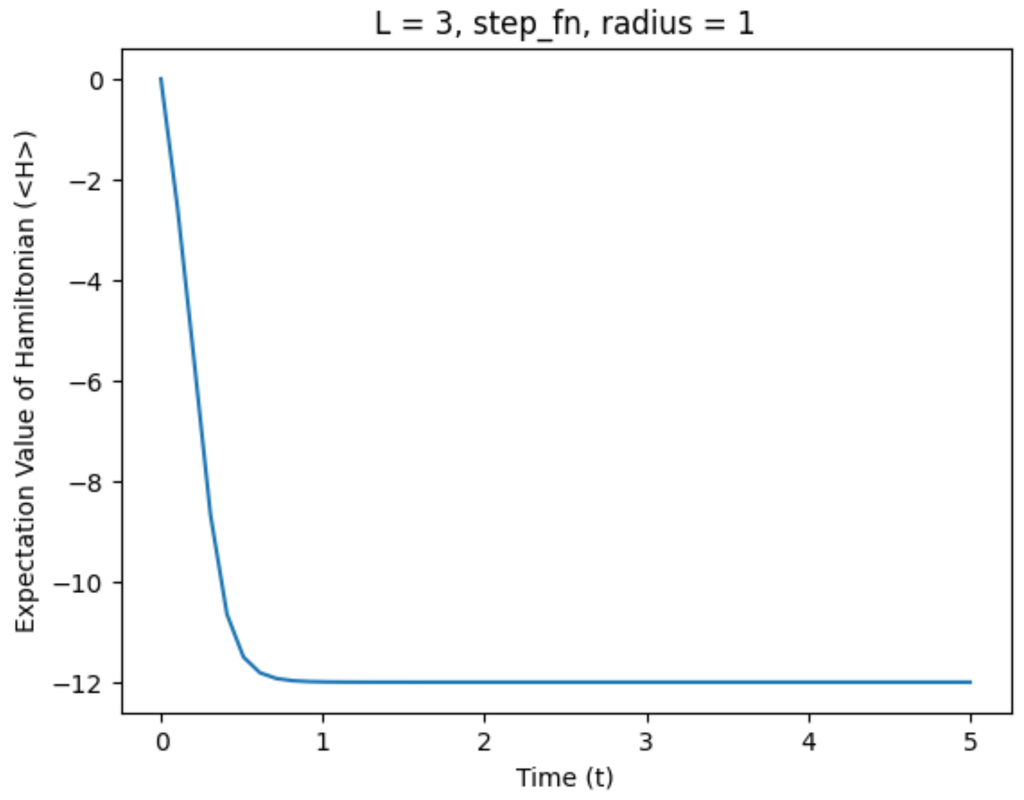
QuSpin (using pre-defined functions in the package)





Numpy/SciPy (using Tamra's libraries + my code)

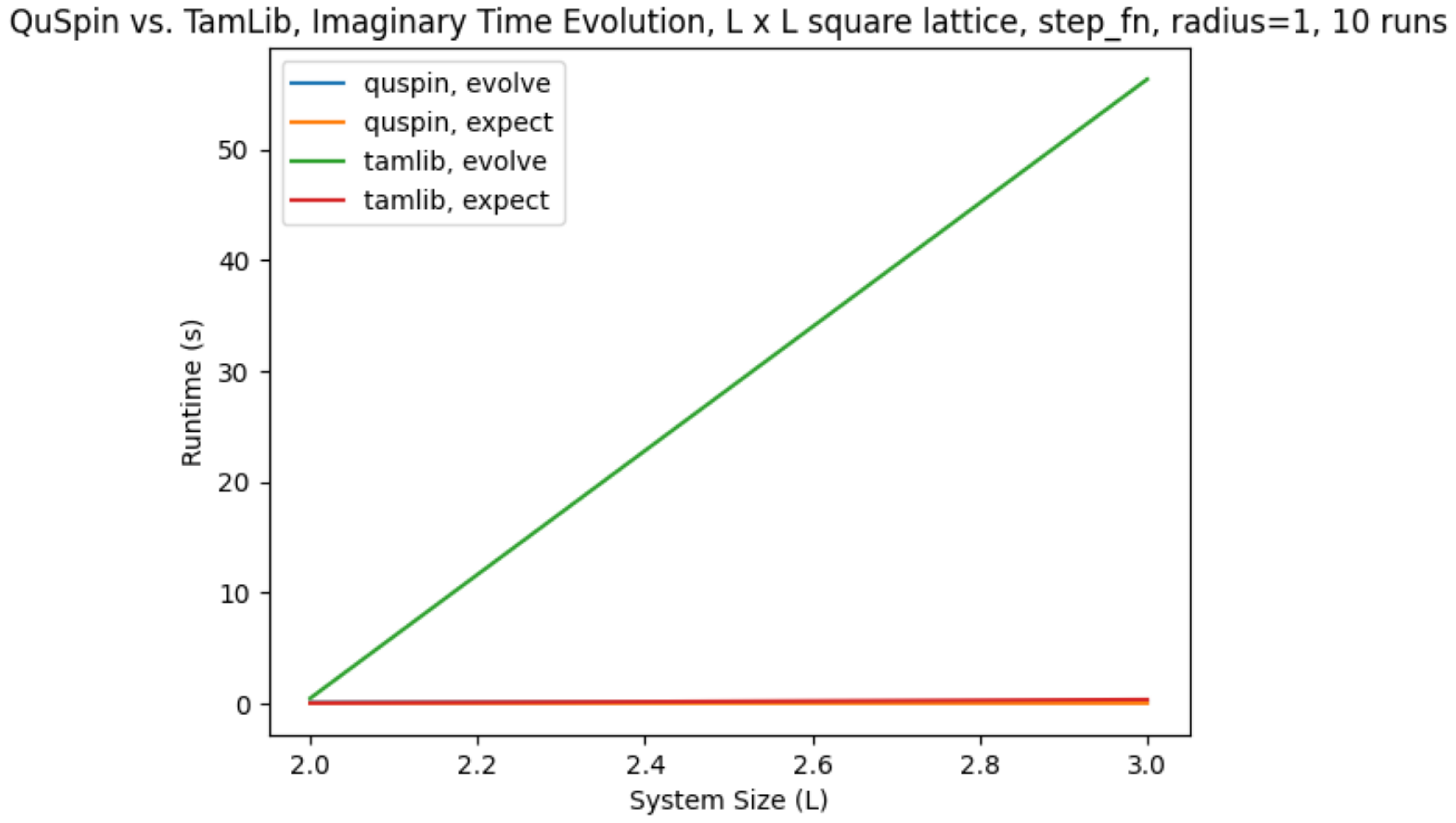




Benchmarking: QuSpin vs. NumPy/SciPy/TamLib

Runtimes over 10 total runs each:

QuSpin	2 x 2	3 x 3
Time Evolution	0.0726437568664551	0.142022371292114
Hamiltonian Expectation	0.00423908233642578	0.00609707832336426
NumPy/ SciPy/TamLib		
Time Evolution	0.457217693328857	56.3067576885223
Hamiltonian Expectation	0.0144739151000977	0.332910060882568



Optimization Method: Variational Quantum Eigensolver (VQE)

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

== Classical optimization ==

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

  == Quantum sub-routine ===

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

- Update parameter $\overrightarrow{\theta}$:= optimizationStep($\overrightarrow{\theta}$)
- Return parameters that minimize objective: $\overrightarrow{\theta} = \min\left(\left\langle \psi_f(\overrightarrow{\theta}) \middle| \hat{H} \middle| \psi_f(\overrightarrow{\theta}) \right\rangle\right)$

Quantum Approximate Optimization Algorithm (QAOA)

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

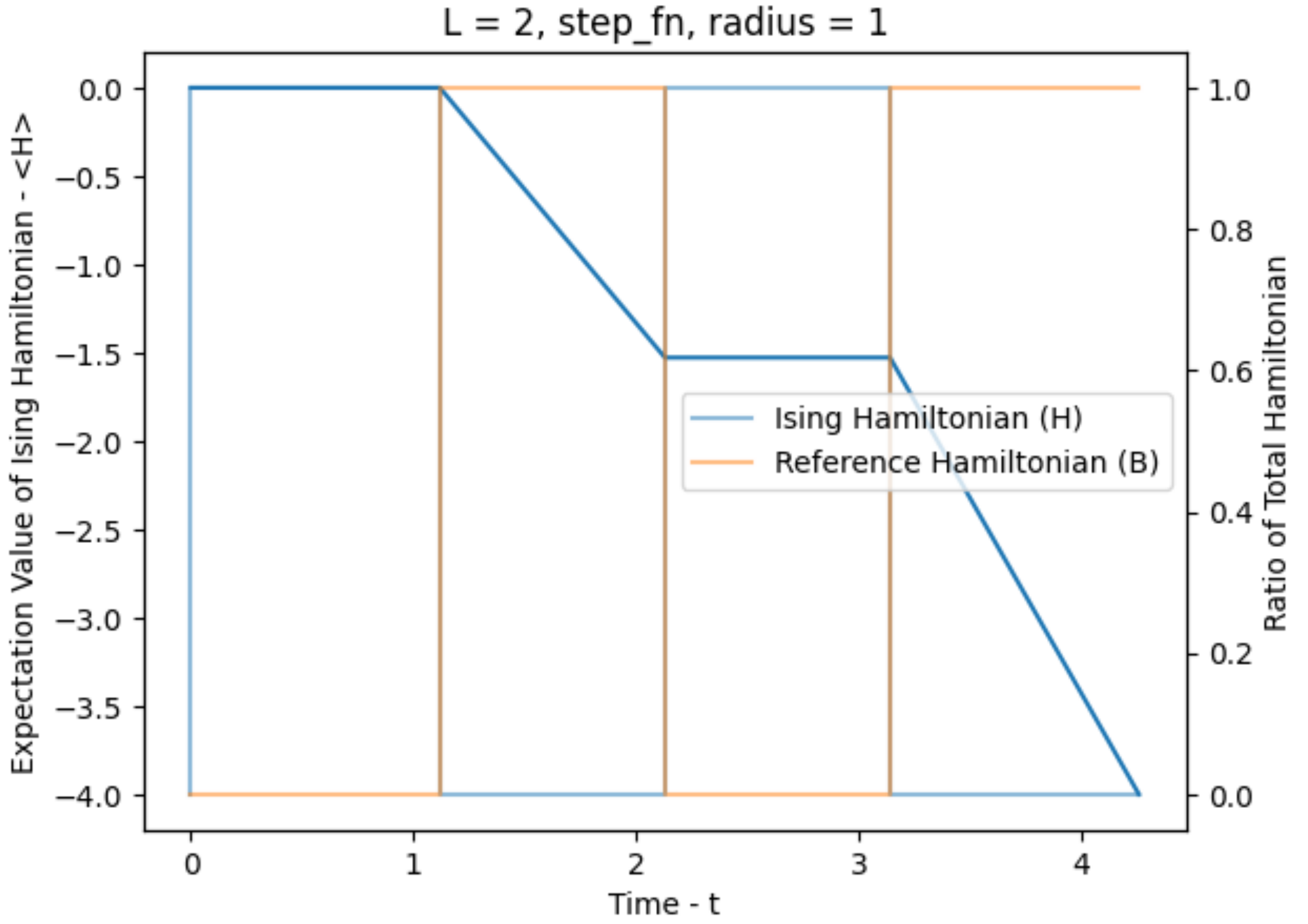
Random initial state, e.g. ground state of $\hat{B}(\sigma)$: $\left|\psi_0\right\rangle = \left| + \right\rangle_{N-1} \otimes \ldots \otimes \left| + \right\rangle_0$

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

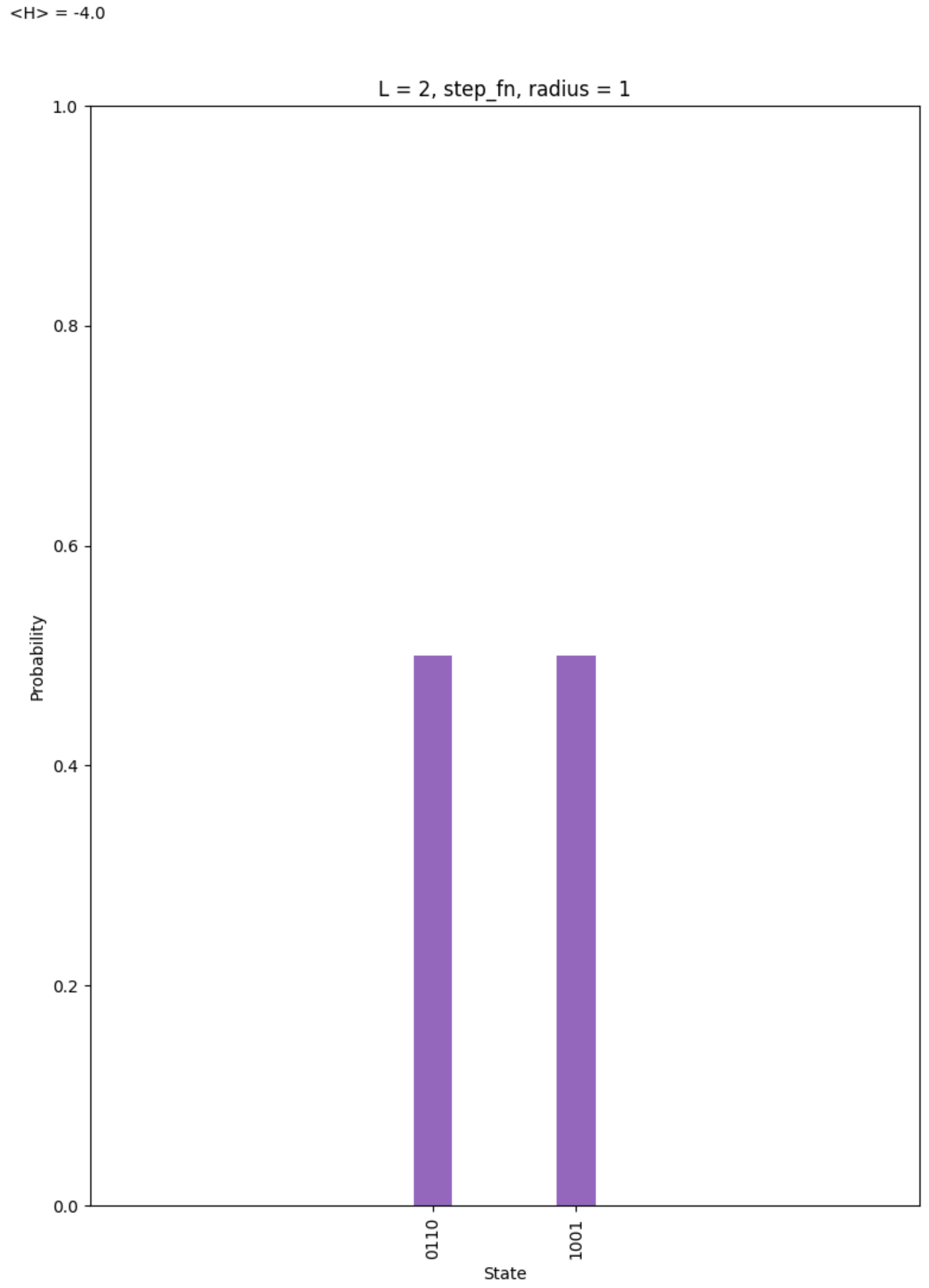
Final state: $\left|\psi_f(\overrightarrow{\beta}, \vec{\gamma})\right\rangle = \hat{U}(\overrightarrow{\beta}, \vec{\gamma})\left|\psi_0\right\rangle$

Parameters: α, $\overrightarrow{\beta}, \vec{\gamma}$

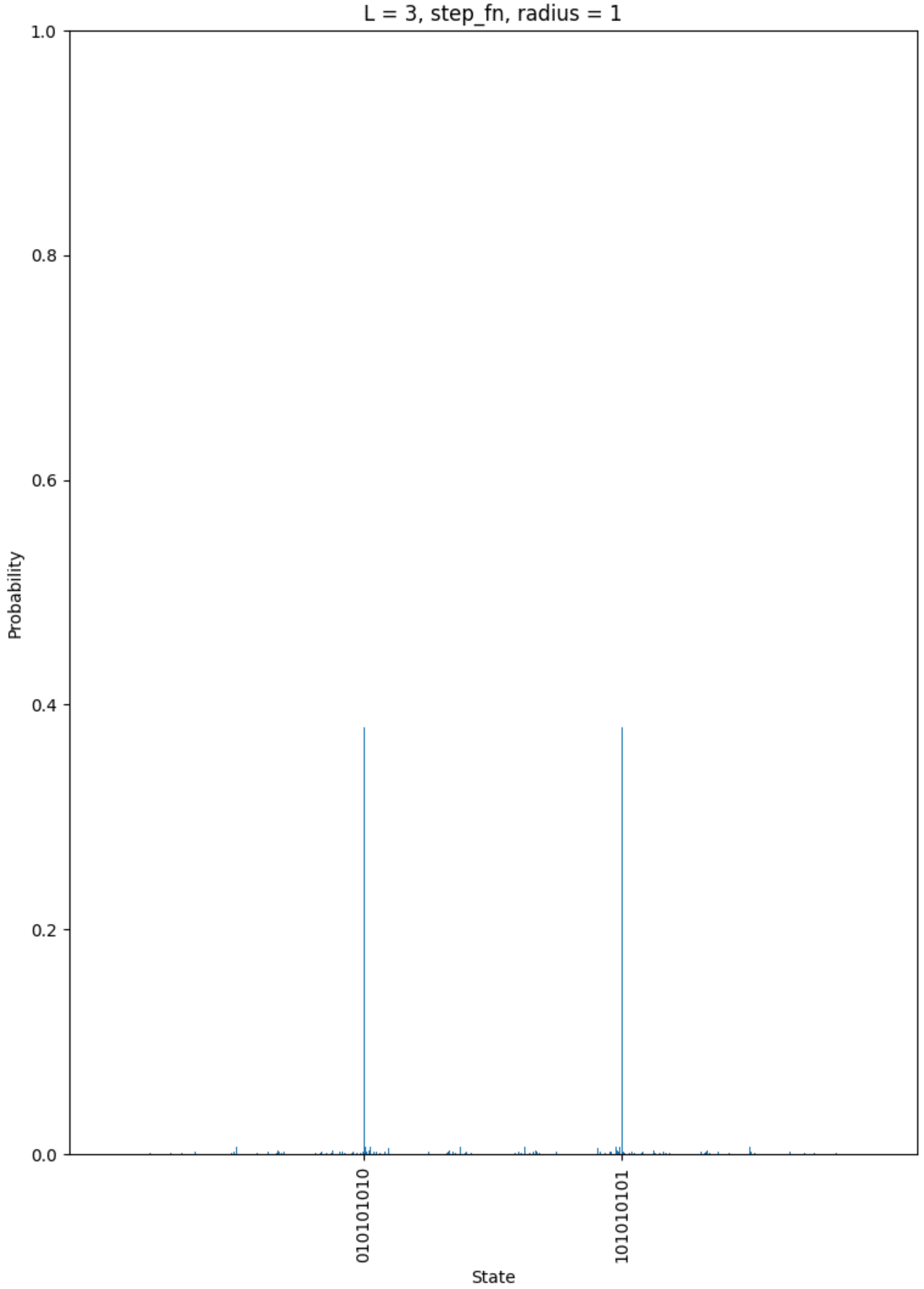
Objective to minimize: $\left\langle\psi_f(\overrightarrow{\beta}, \vec{\gamma})\middle|\hat{H}\middle|\psi_f(\overrightarrow{\beta}, \vec{\gamma})\right\rangle$

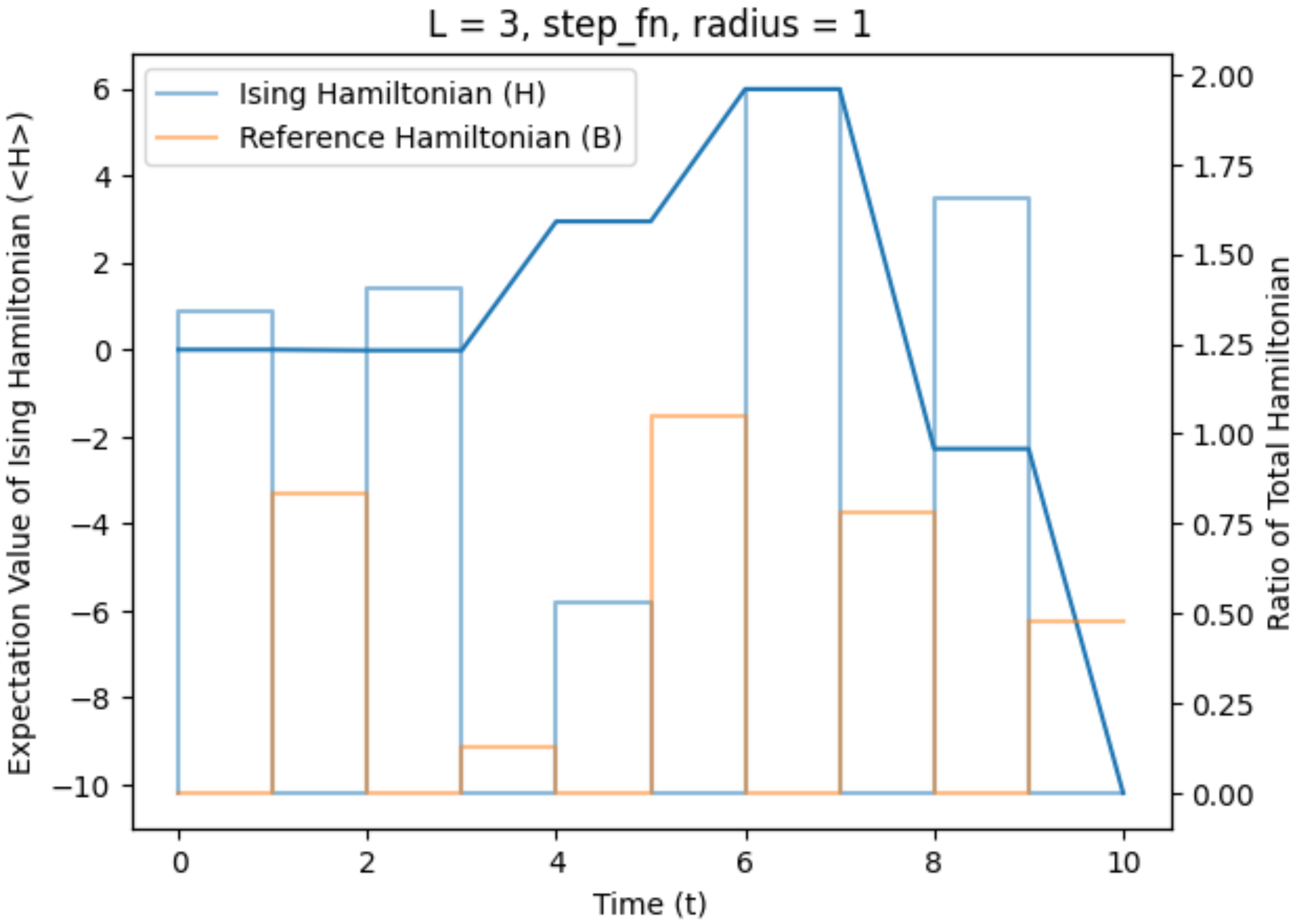


Optimization: $\overrightarrow{\beta}, \vec{\gamma} = \text{VQE}\left(\text{ansatz} = \left|\psi_f(\overrightarrow{\beta}, \vec{\gamma})\right\rangle, \text{operator} = \hat{H}\right)$



<H> = -10.2


L = 3, step_fn, radius = 1
Probability
1.0
0.8
0.6
0.4
0.2
0.0
010101010
101010101
State


L = 3, step_fn, radius = 1
Ising Hamiltonian (H)
Reference Hamiltonian (B)
Expectation Value of Ising Hamiltonian (<H>)
Ratio of Total Hamiltonian
Time (t)
6
4
2
0
−2
−4
−6
−8
−10
2.00
1.75
1.50
1.25
1.00
0.75
0.50
0.25
0.00
0
2
4
6
8
10

Adiabatic Quantum Evolution (AQE)

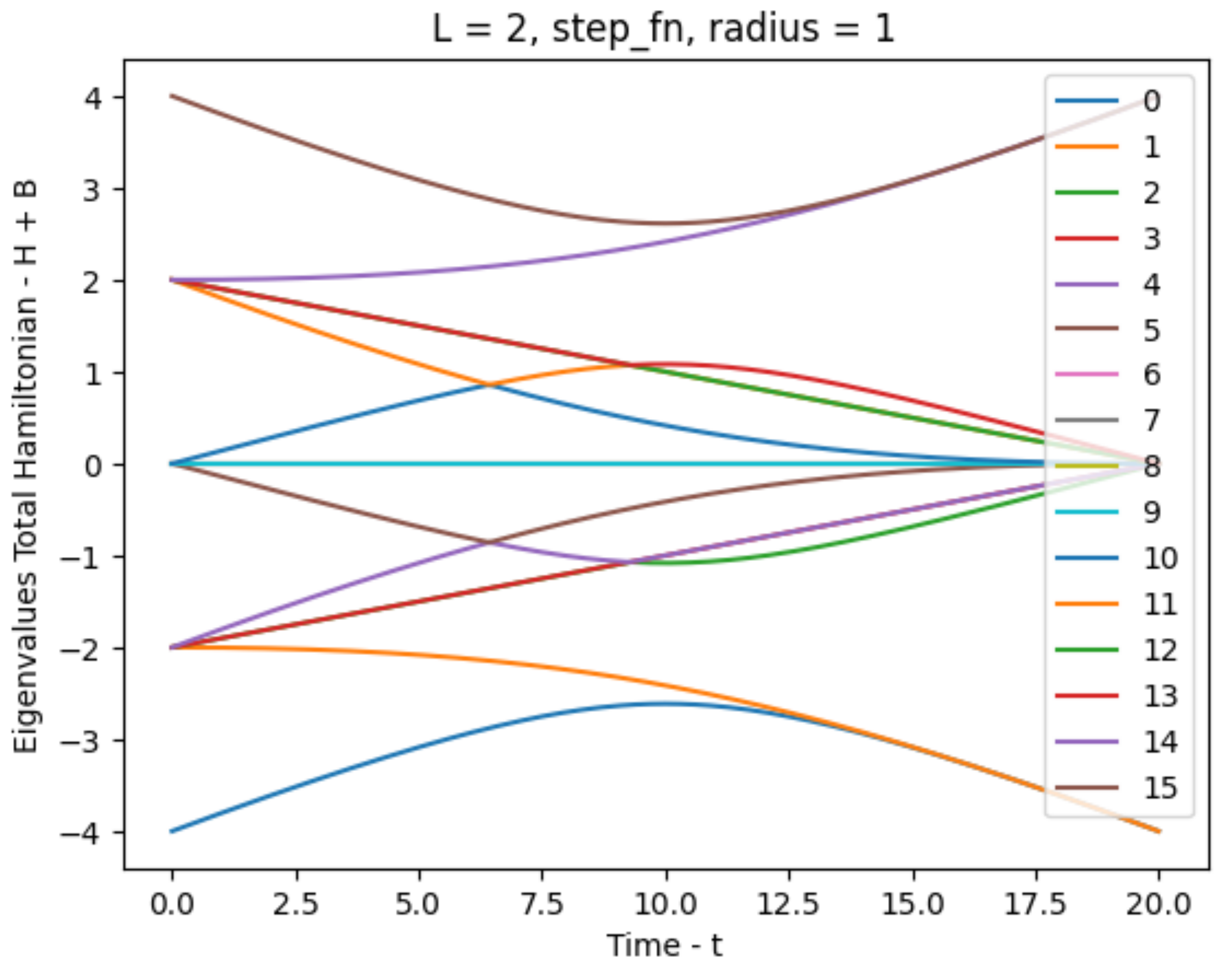
Ising Interaction Hamiltonian: $\hat{H}(\sigma) = -\sum_{ij} J_{ij}\sigma_i^z\sigma_j^z$, Reference Hamiltonian: $\hat{B}(\sigma) = -\sum_{i} \sigma_i^x$

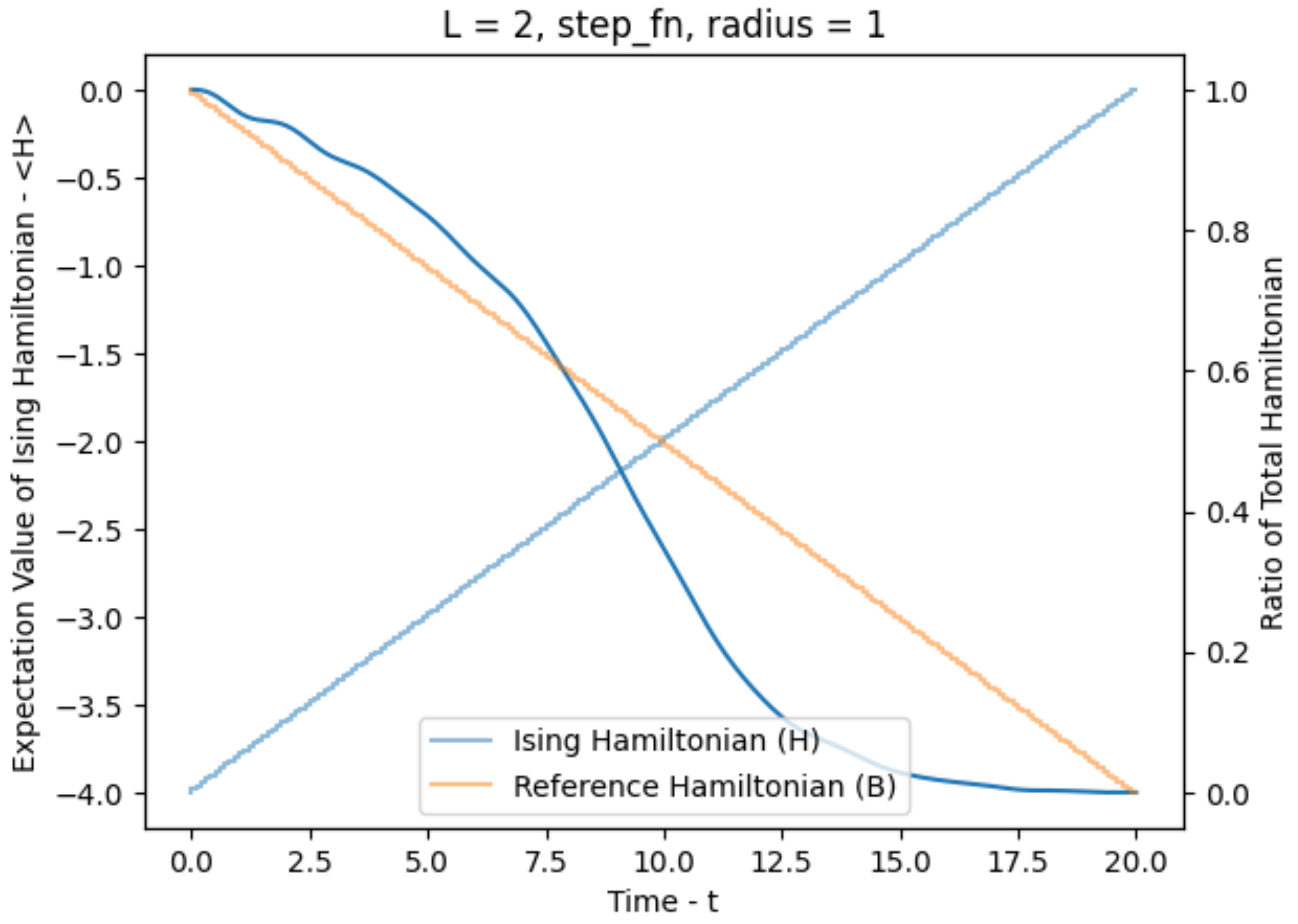
Evolution Hamiltonian: $\hat{H}(\tau) = (1-\tau)\hat{B} + \tau\hat{H}, \tau \in [0,1]$

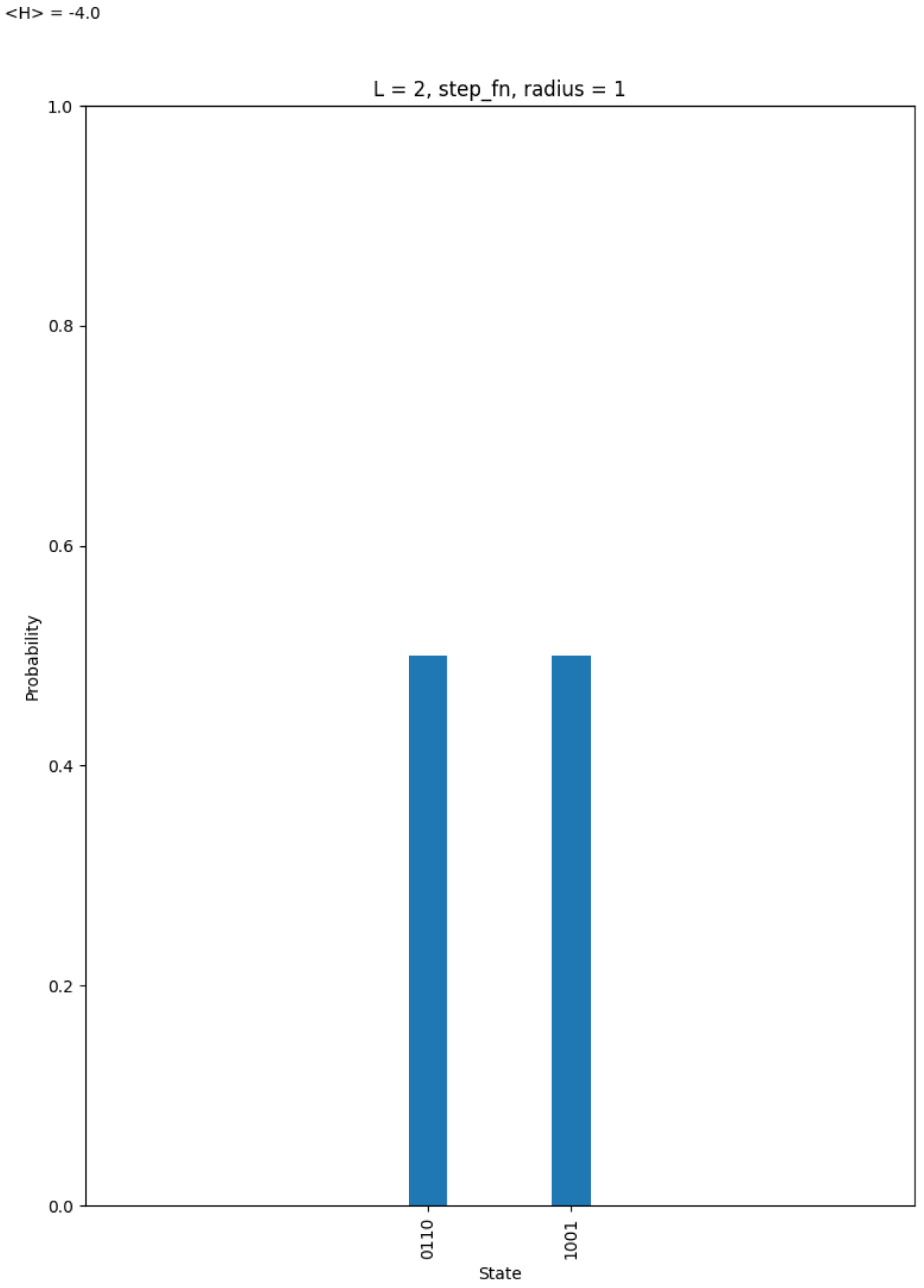
Initial state = ground state of $\hat{B}(\sigma)$: $\left|\psi_0\right\rangle = |+\rangle_{N-1} \otimes \ldots \otimes |+\rangle_0$

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

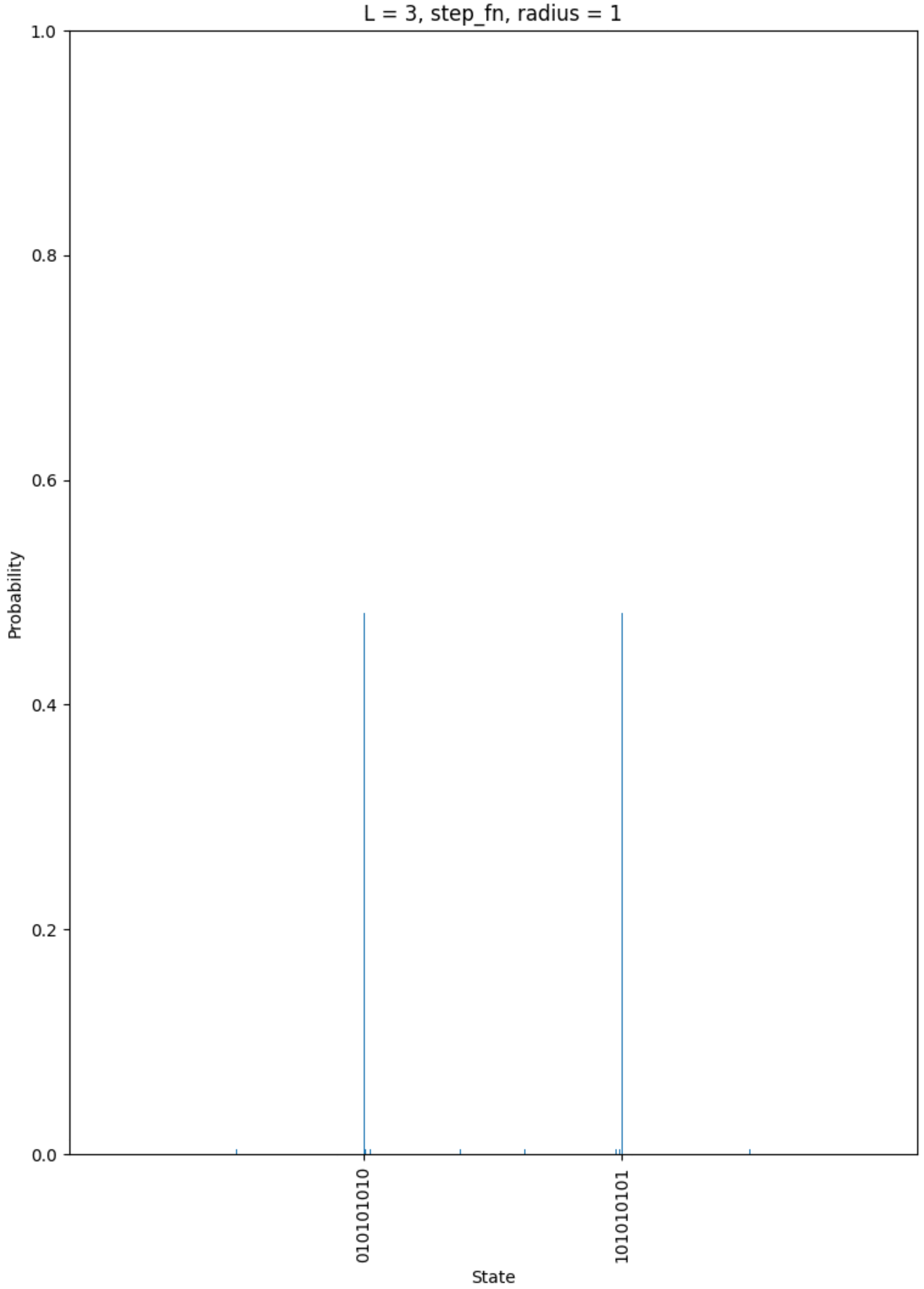
Objective to minimize: $\left\langle \psi_f \middle| \hat{H} \middle| \psi_f \right\rangle$

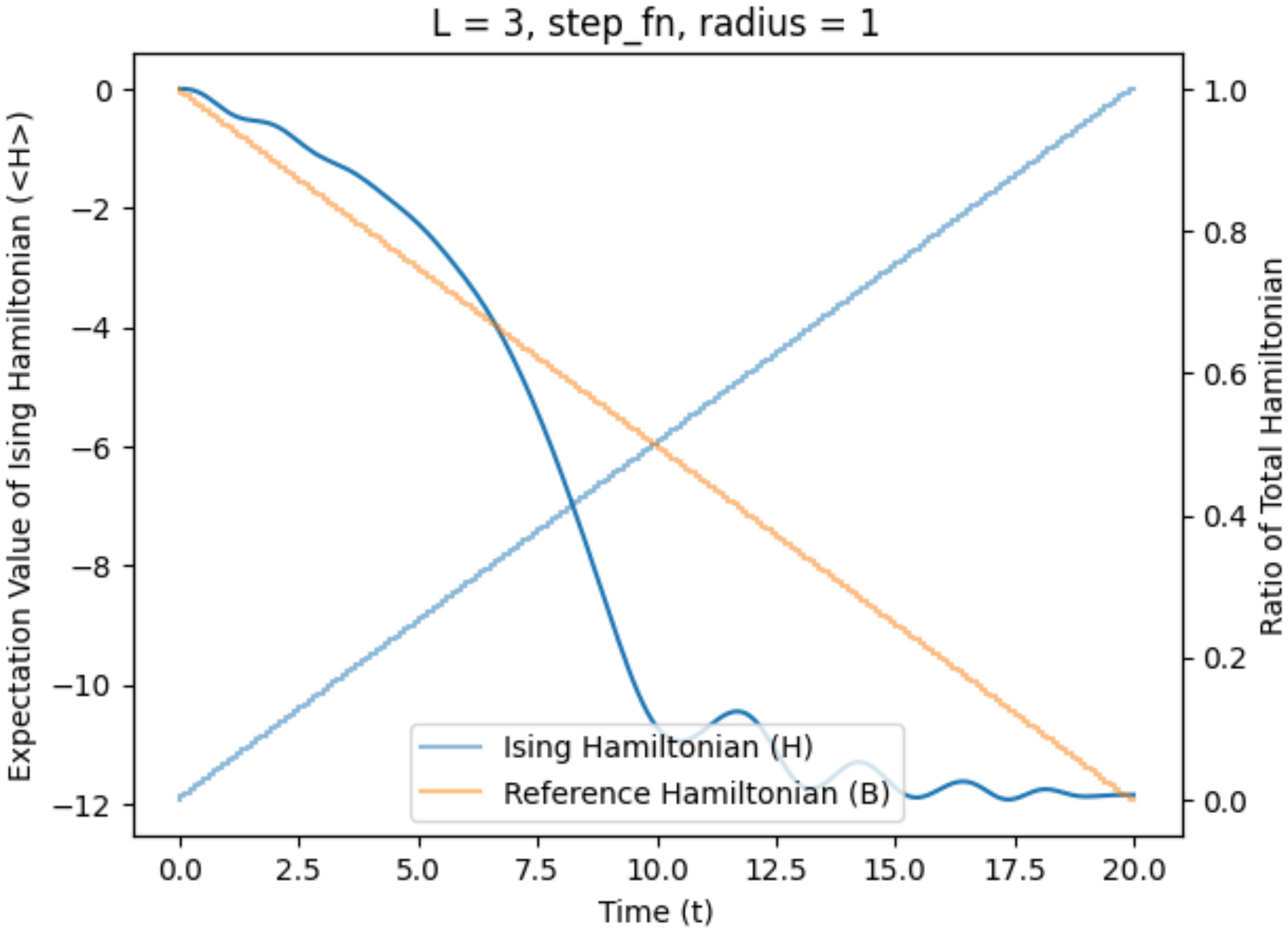






<H> = -11.8


L = 3, step_fn, radius = 1
Probability
1.0
0.8
0.6
0.4
0.2
0.0
010101010
101010101
State


L = 3, step_fn, radius = 1
Expectation Value of Ising Hamiltonian (<H>)
Ratio of Total Hamiltonian
Time (t)
Ising Hamiltonian (H)
Reference Hamiltonian (B)
0
−2
−4
−6
−8
−10
−12
0.0
2.5
5.0
7.5
10.0
12.5
15.0
17.5
20.0
1.0
0.8
0.6
0.4
0.2
0.0

Next Steps

- Optimize circuit depth for QAOA (given optimal angles by VQE optimization)
  - Evaluation metric: ground state fidelity (similar to corresponding metric in classical)
  - Evaluation parameters:
    - Circuit depth (number of pulse sequences, α)
    - Integrated interaction strength x time ($\sum_{i=0}^{\alpha-1} \beta_i$)
- Optimize circuit depth for VQE optimization
  - Evaluation parameter: circuit depth (number of pulse sequences, α)
  - Bound / add regularization term penalizing integrated interaction strength x time ($\sum_{i=0}^{\alpha-1} \beta_i$) during optimization
- Explore DTWA for simulating larger quantum systems
- Policy Gradient Based Quantum Approximate Optimization Algorithm (May 2020) ?

Bibliography

- https://www.cs.cmu.edu/afs/cs/academic/class/15854-f05/www/scribe/lec02.pdf
- http://www.mit.edu/~ilkery/papers/MetropolisHastingsSampling.pdf
- https://mathworld.wolfram.com/SimulatedAnnealing.html
- https://arxiv.org/pdf/1505.03068.pdf
- https://doi.org/10.4236/am.2017.88090
- https://iopscience.iop.org/article/10.1088/0305-4470/31/41/011/meta
- https://grove-docs.readthedocs.io/en/latest/vqe.html
- https://grove-docs.readthedocs.io/en/latest/qaoa.html
- https://arxiv.org/pdf/1304.3061.pdf
- https://iopscience.iop.org/article/10.1088/1367-2630/18/2/023023/ampdf
- https://scipost.org/SciPostPhys.2.1.003/pdf
- https://scipost.org/SciPostPhys.7.2.020/pdf
- http://large.stanford.edu/courses/2008/ph372/behroozi2/
- http://weinbe58.github.io/QuSpin/index.html
- https://arxiv.org/pdf/1508.07314.pdf
- https://paramekanti.weebly.com/uploads/1/1/2/8/11287579/atan_paper.pdf
- http://users.ox.ac.uk/~phys1116/msm2.pdf
- https://www.math.arizona.edu/~tgk/541/chap1.pdf
- https://arxiv.org/pdf/2002.01068.pdf