Searching for a Connection between Maximum Entropy and the Arrow of Time

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The arrow of time & the laws of physics

- The direction time flows in is something we can easily see in the world around us
- However, not all of physics reflects this reality
- Two different domains:

Microscopic

- Reversible and symmetrical in time
- Small-scale
- Examples:
  - Photon emission

Macroscopic

- Irreversible and asymmetrical in time
- Probabilistic
- Large-scale
- Examples:
  - Heat transfer

Our goal

- To find a resolution to the conflict between the two pictures
- How? By simulating the Ising model

What is the Ising model?

- One of the most thoroughly-researched statistical models in physics
- Consists of a lattice of spin sites that point either up or down
- Energy Hamiltonian:

$$E = -J \sum_{<i,j>} s_i s_j - B \sum_i s_i$$

- Energy change from flipping a site's orientation:

$$|\Delta E| = 2zJ$$

The lattice visualised

- Small up-spin lattice:

↑↑↑

- Total energy is -3
- Flip middle spin:

↑↓↑

- New energy is 1
- Useful to think of in terms of bonds

The Metropolis algorithm

- First developed by Nicholas Metropolis in 1953 to describe hard-sphere gases
- Monte Carlo method that uses transition probabilities to simulate the Ising model
- Steps:
    1. Select a random site in the lattice
    2. If the energy change of a spin-flip would be negative, accept the flip
    3. If it would be positive, accept the flip with probability $P = e^{-J \Delta E}$
    4. Repeat

The Creutz algorithm

- Deterministic counterpart of the Metropolis algorithm
- Instead of a probabilistic thermal bath, it uses a kinetic energy ‘demon’
- When a spin-flip happens, energy is transferred between the system and its demons
    - Upward transitions are only possible if the demons have enough energy for it

The Creutz algorithm: dynamic bond formation

- A variation in which the bonds between lattice sites are allowed to form and break
- Similar to a modification Creutz described to his original algorithm in 1985, but not identical
- Varies the lattice coordination number z of a site between 0, 1, and 2
- In terms of the algorithm, there is an extra step at the end checking whether the demons have enough energy to break or form a bond
- Remains reversible

The Creutz algorithm: variable timescale

- Different conditions for different parts of the simulation: bonds were frozen for the middle third, dynamic otherwise
- Effectively random bond structure
- Similar behavior has been observed in glass molecules
- Purpose is to measure the effect of frozen bonds on the system's maximum entropy

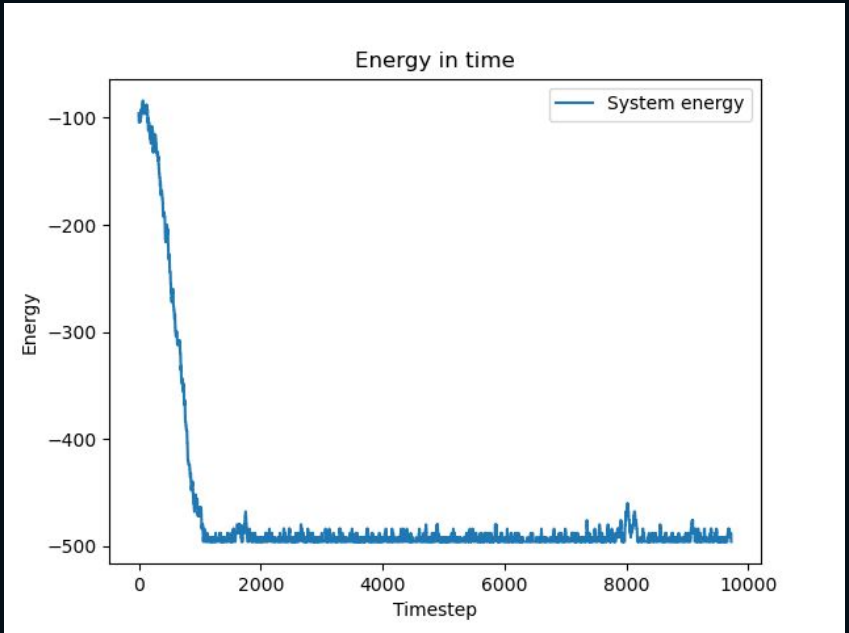
$$p_{n+1}/p_n = e^{-J\Delta E}$$

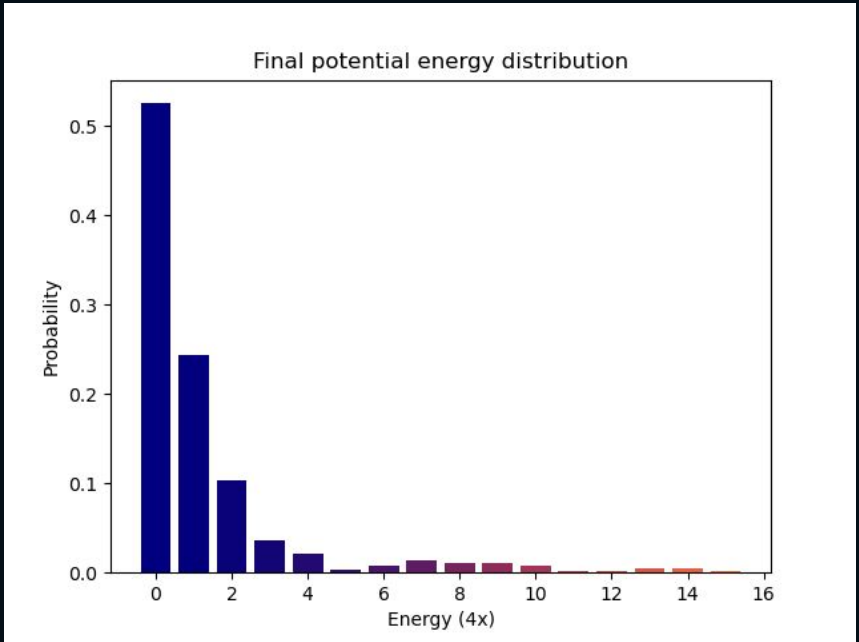
$$\ln p_{n+1} - \ln p_n = -J = \Delta \ln p$$

Implementing the model & algorithms

- Python programming language
- Four primary considerations
  - Generality
  - Flexibility
  - Readability
  - Speed

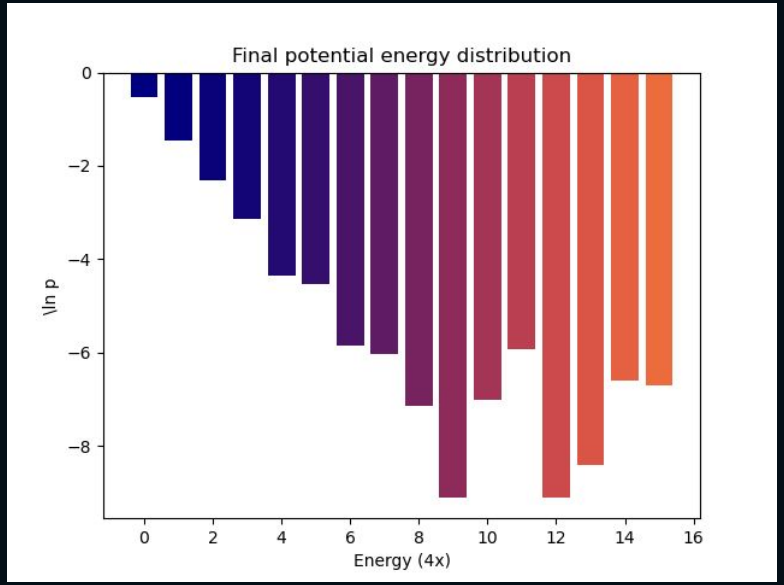
The Metropolis algorithm: results



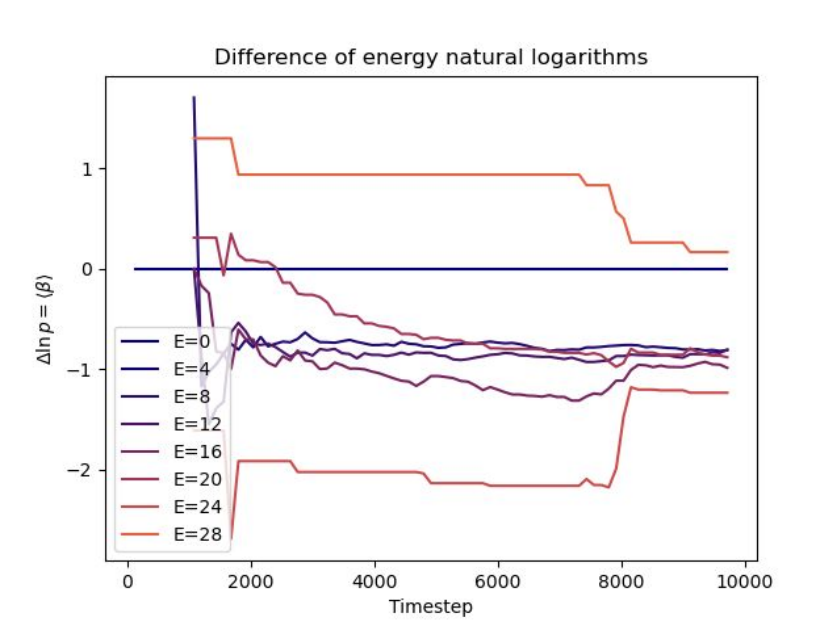


Temperature: $1/J\square = 2.5$

The Metropolis algorithm: results



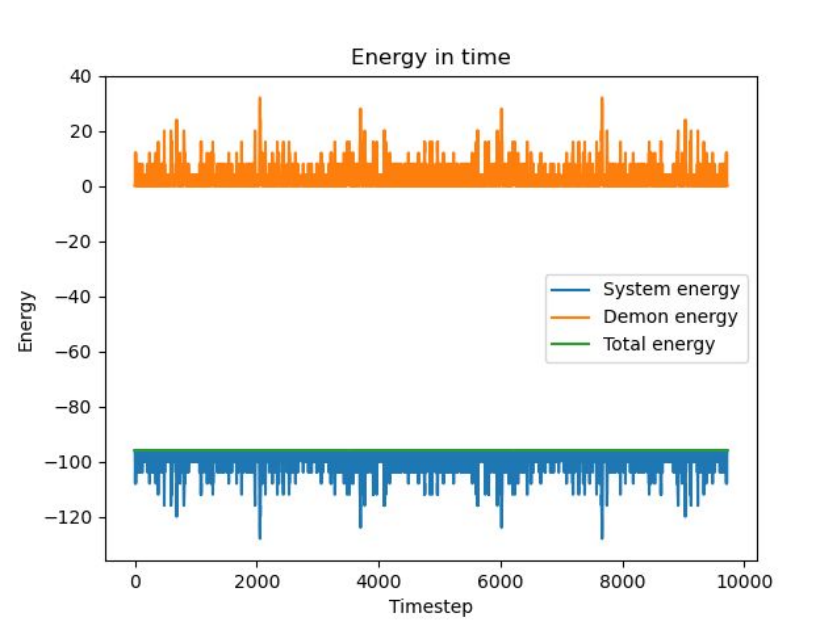
The Metropolis algorithm: results

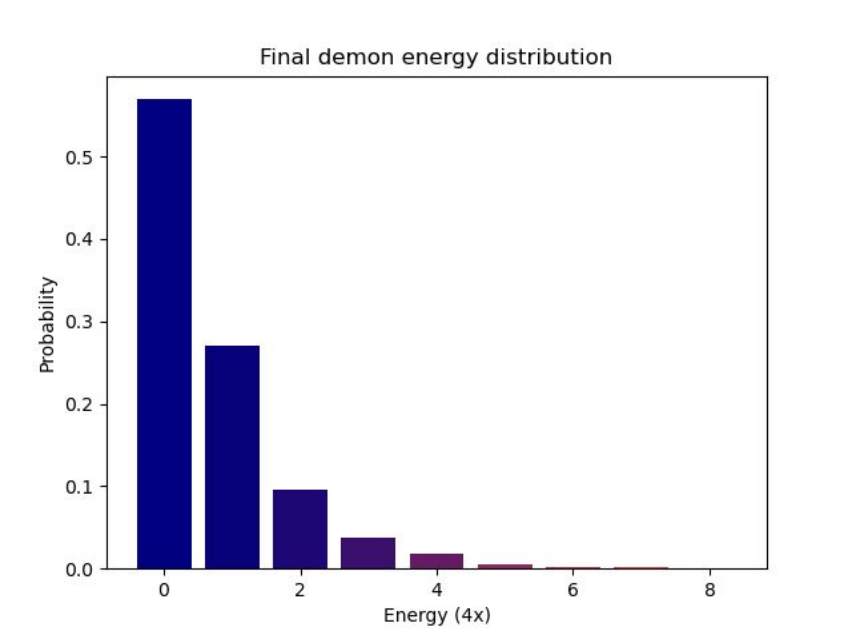


Energy	Temperature
4	—
8	5.150
12	4.596
16	3.570
20	4.904
24	2.211
28	-6.027

Average: $1/J\square = 4.1 \pm 1.2$

The Creutz algorithm: results





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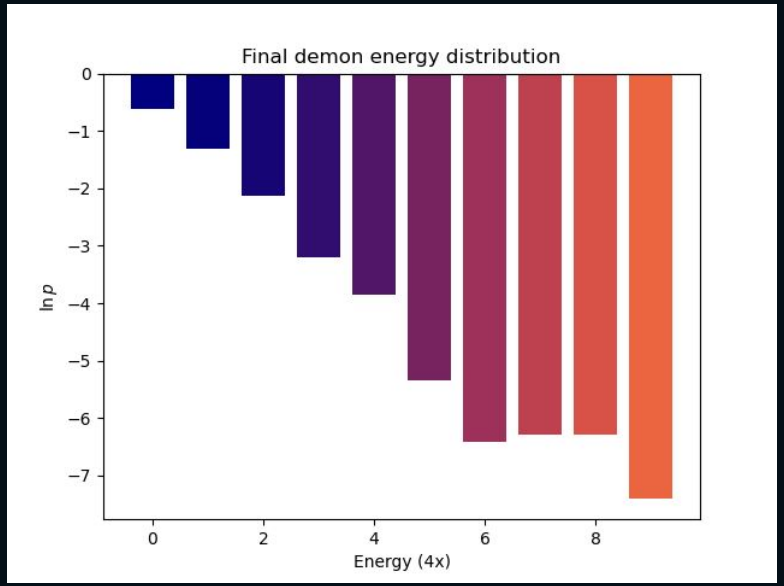

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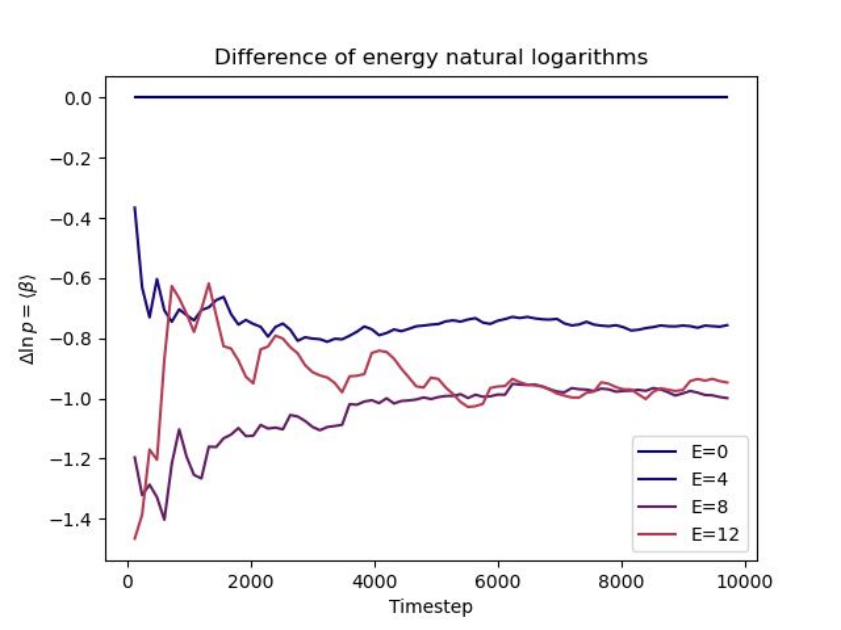
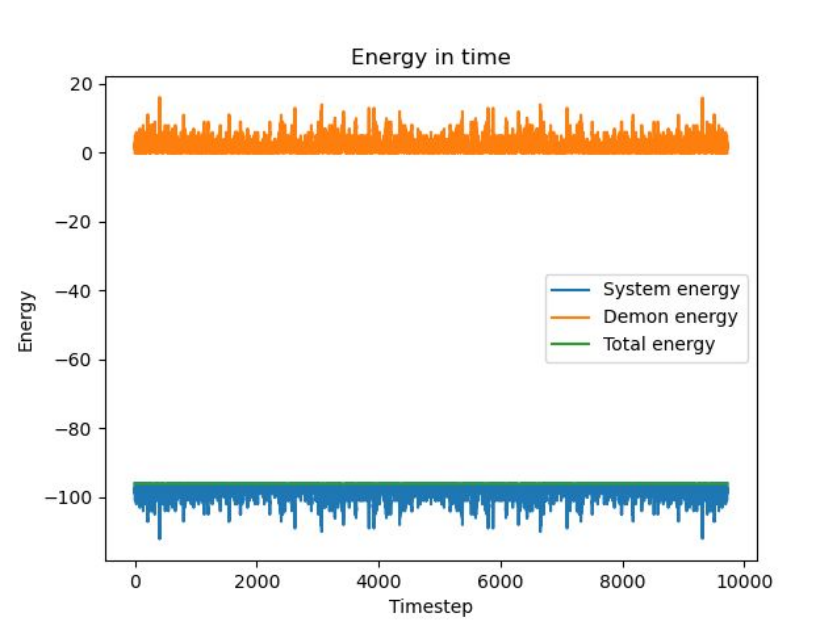
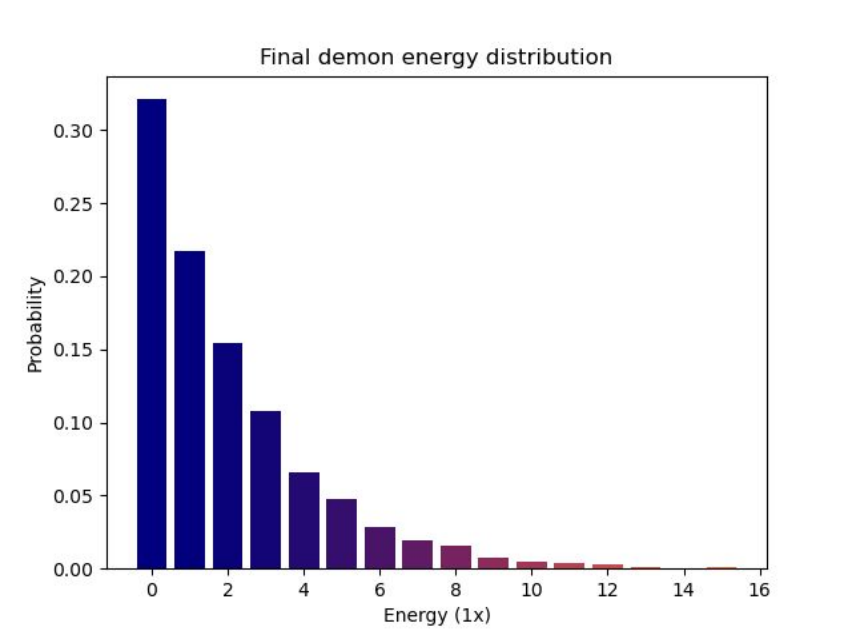


Energy	Temperature
4	5.326
8	4.087
12	4.127

Average: $1/J\square = 4.5 \pm 0.7$

The Creutz algorithm (dynamic bonds): results





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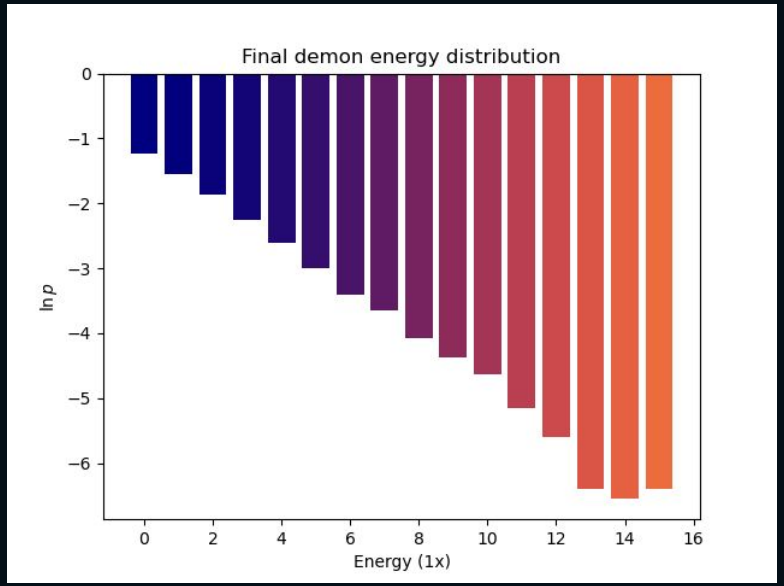

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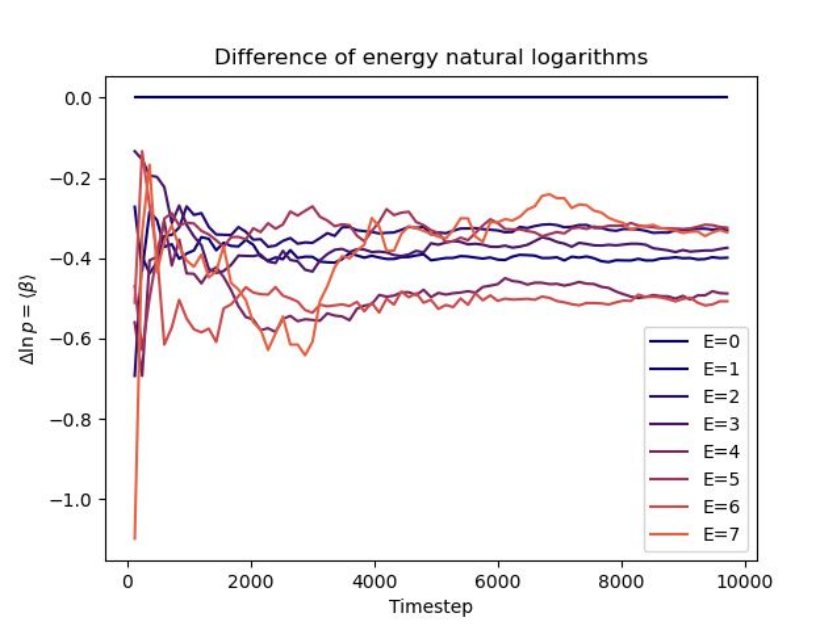
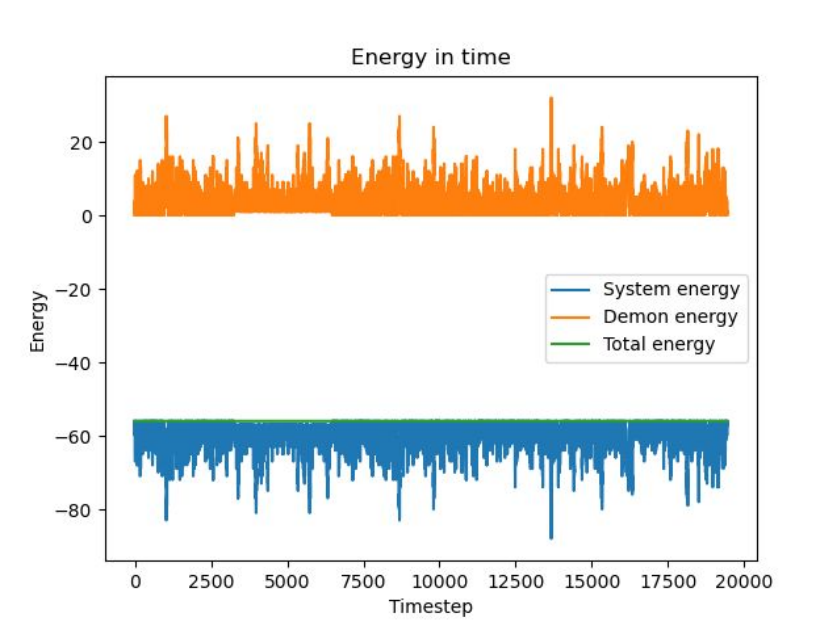
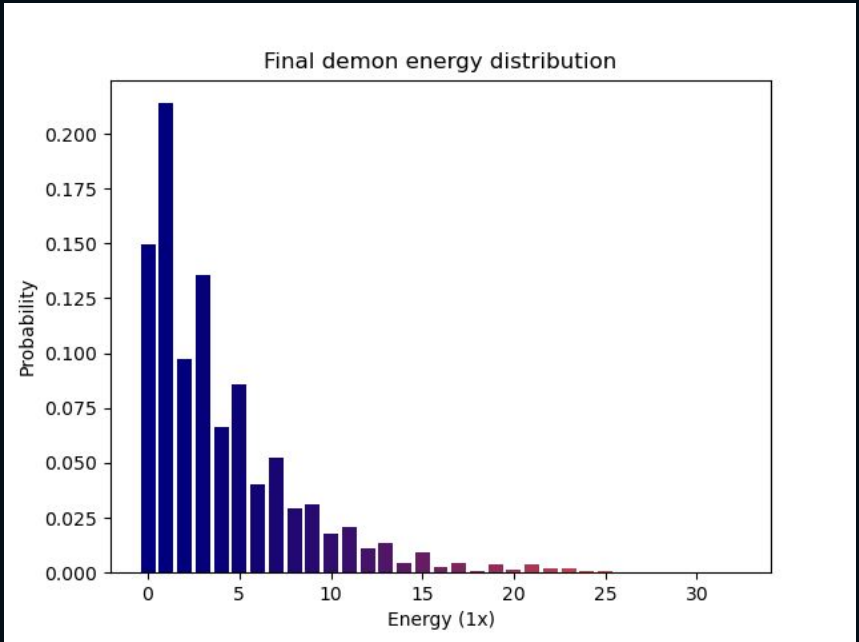


Energy	Temperature
1	2.498
2	3.051
3	2.713
4	2.086
5	3.047
6	1.976
7	3.240

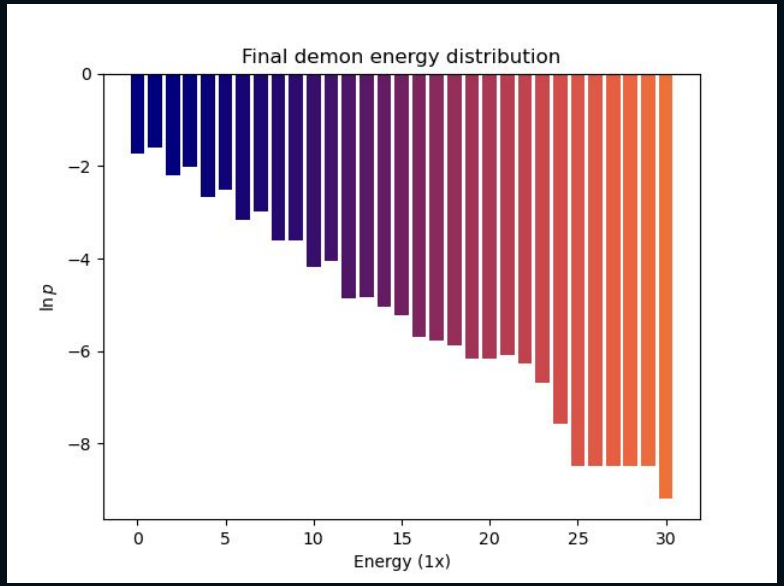
Average: $1/J\square = 2.7 \pm 0.5$

The Creutz algorithm (variable timescale): results

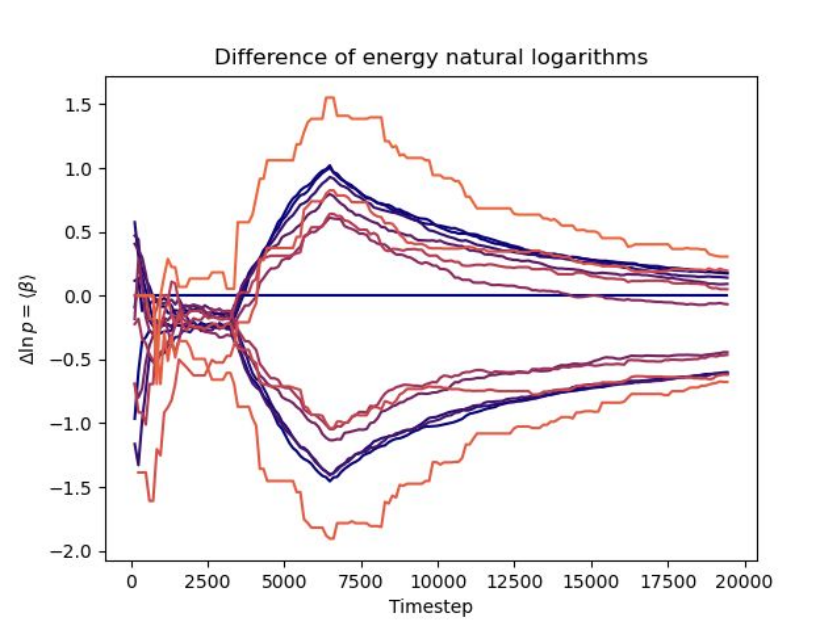


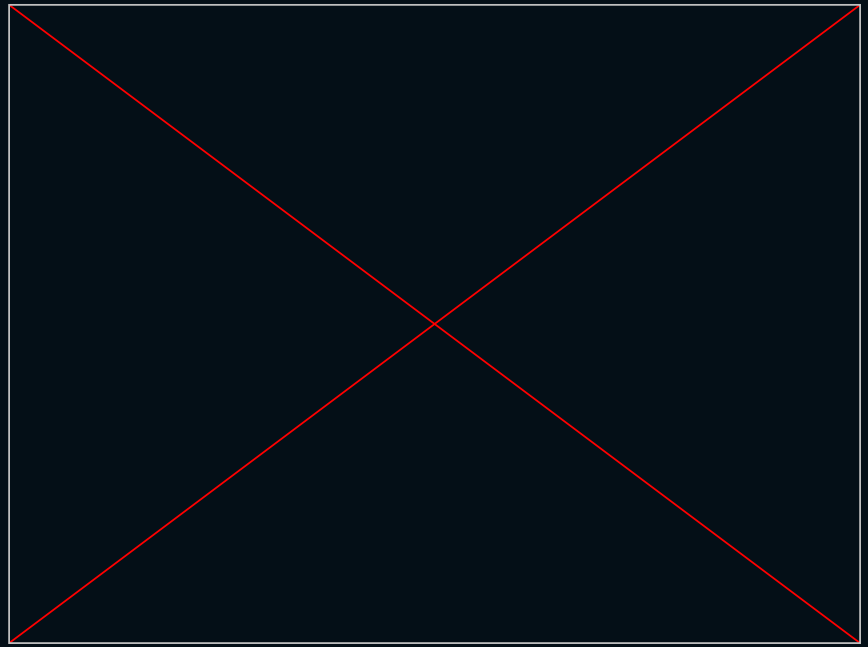


The Creutz algorithm (dynamic bonds): results



The Creutz algorithm (variable timescale): results





Results of the Metropolis algorithm simulation

- As expected, the model favors low energy states and generates the Boltzmann distribution
- However, the distribution was skewed for the spins due to the multiplicity of an energy macrostate
    - We could have adjusted the results to account for this, but we elected not to
- Temperature results were limited by simulation time and lattice size
- We can confidently conclude that our implementation of the Ising model is accurate

Results of the Creutz algorithm

- It was reversible in time and generated the Boltzmann distribution, as expected
- The temperatures were a little high, but still in good agreement with the Metropolis simulation

Results of the Creutz algorithm (dynamic bonds)

- The dynamic bond Creutz algorithm behaved just as well, also generating the Boltzmann distribution and being reversible
- The temperature was low compared to the static bond algorithm’s, but not concerningly so
    - Closer to Metropolis, which is our benchmark for accuracy

Results of the Creutz algorithm (variable timescale)

- The two algorithms used in the simulation generate the Boltzmann distribution on their own, but not together
- The three epochs of the simulation corresponded clearly with adherence to the Boltzmann distribution
- From the perspective of the second law of thermodynamics, these results are quite interesting
    - We cannot yet make any definitive conclusions, though

Our conclusions

- Our implementation of the Ising model, as well as the Metropolis and Creutz algorithms, behaved in accordance with expectations
- The results generated by the variable timescale Creutz algorithm very much suggest that there exists a connection between maximum entropy and bond freezing, but we cannot state that with certainty yet
    - Still highly promising
- Further research into the subject would be very worthwhile

References

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