1 Introduction

The Creutz algorithm [1] was implemented as another example of a Monte Carlo method to simulate a microcanonical ('NVE') ensemble for the 3D Ising model. We focus our experiment on energy E and calculate temperature T of the system from it in two different ways.

2 Algorithm Description

The implemented Creutz algorithm works as follows:

- initialize 3d Ising grid with all spins aligned down.
- randomly pick a site: If flipping its spin increases total energy, do so; repeat until system reaches target energy E
- release demon once system has reached target energy: Demon has energy $E_d = 0$ with $E_{max} = 0.05 \cdot E$.
- demon jumps to random site and calculates ΔE for a potential spin flip: Iff $E_{max} \geq E_d \geq 0$ keep flip.
- recording E_d completes one Monte Carlo step; repeat demon jump until number of steps required

The temperature T then is calculated using two different ways for comparison:
The probability distribution $P(E_d)$ of the demon energy E_d is plotted in a semilog plot. The slope of the linear fit to $P(E_d)$ then equals the inverse temperature β as in equation 1.

$$P(E_d) \approx e^{-\frac{E_d}{k_B T}} \tag{1}$$

For comparison, the temperature is calculated analytically according to equation 2.

$$\frac{k_B T}{J} = \frac{4}{\log(1 + \frac{4J}{<E_d>})} \tag{2}$$

3 Results

The program was implemented as described above and submitted with this report. For all experiments, the coupling constant J was fixed to the simplest ferromagnetic value of $J = 1.0$. Experiments where run for system side lengths $L \in \{10, 20\}$ and average site energies $E \in \{-2.9, -2.5, -2.0, -1.5, -1.0, -0.5\}$ (figures 1 and 2).

Calculated temperatures and plotted temperatures then were plotted for all energies (figures 3 and 4).

4 Discussion

The results for dimensionless temperature T agree almost perfectly between the two calculation methods.
Also, plotting temperatures for several energies in a single plot manages to reproduce the behaviour simulated using the Metropolis algorithm during a previous exercise (figures 3 and 4).

References

[1] Creutz, M.
Microcanonical Monte Carlo Simulation,
Phys. Rev. Lett. American Physical Society. 50 (19): 1411–1414,
1983.

[2] Boettcher, L.,
Computational Statistical Physics - Lecture Notes,
ETH Zurich,
2019.

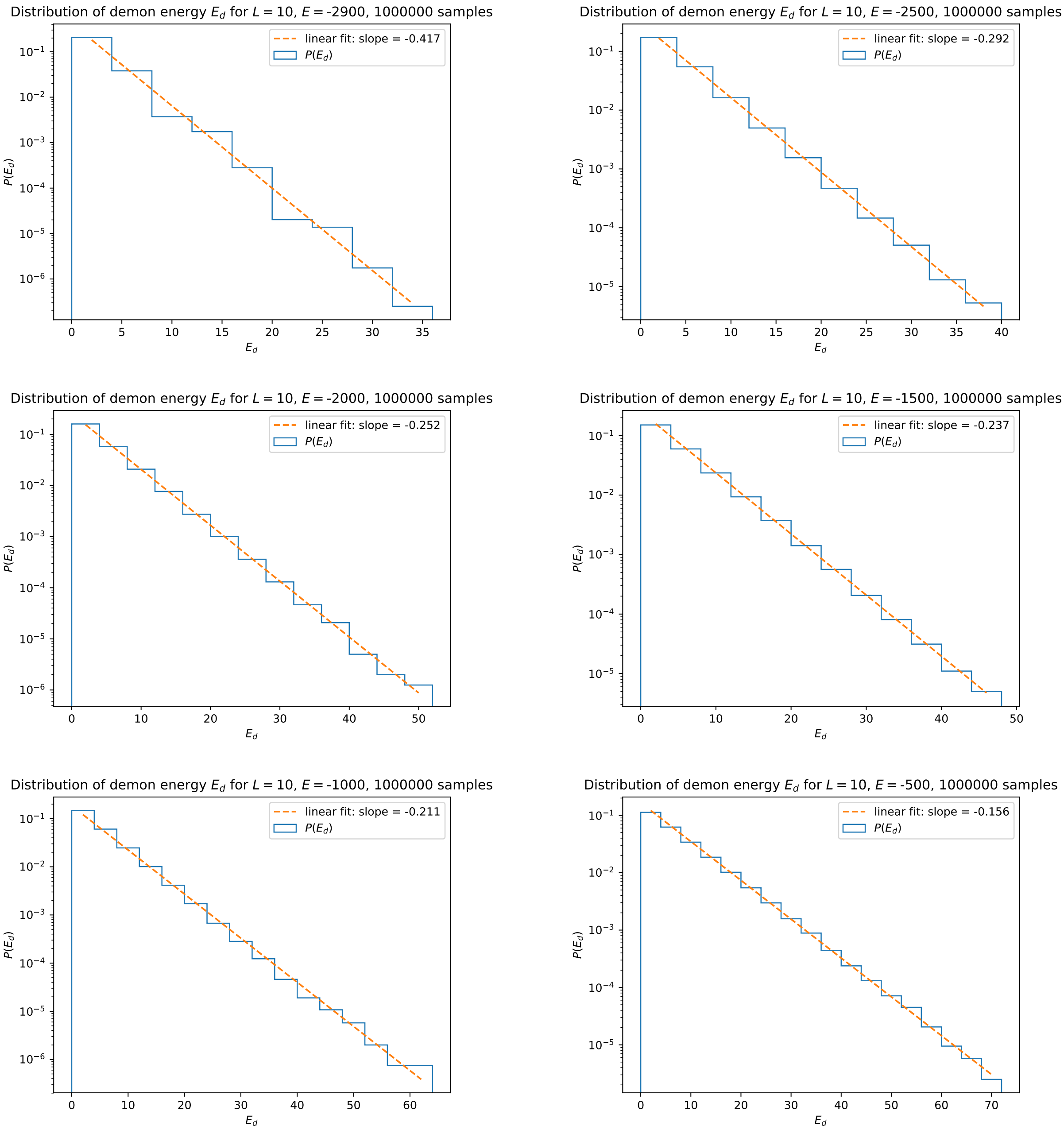

Figure 1: $P(E_d)$ plots for $L = 10$

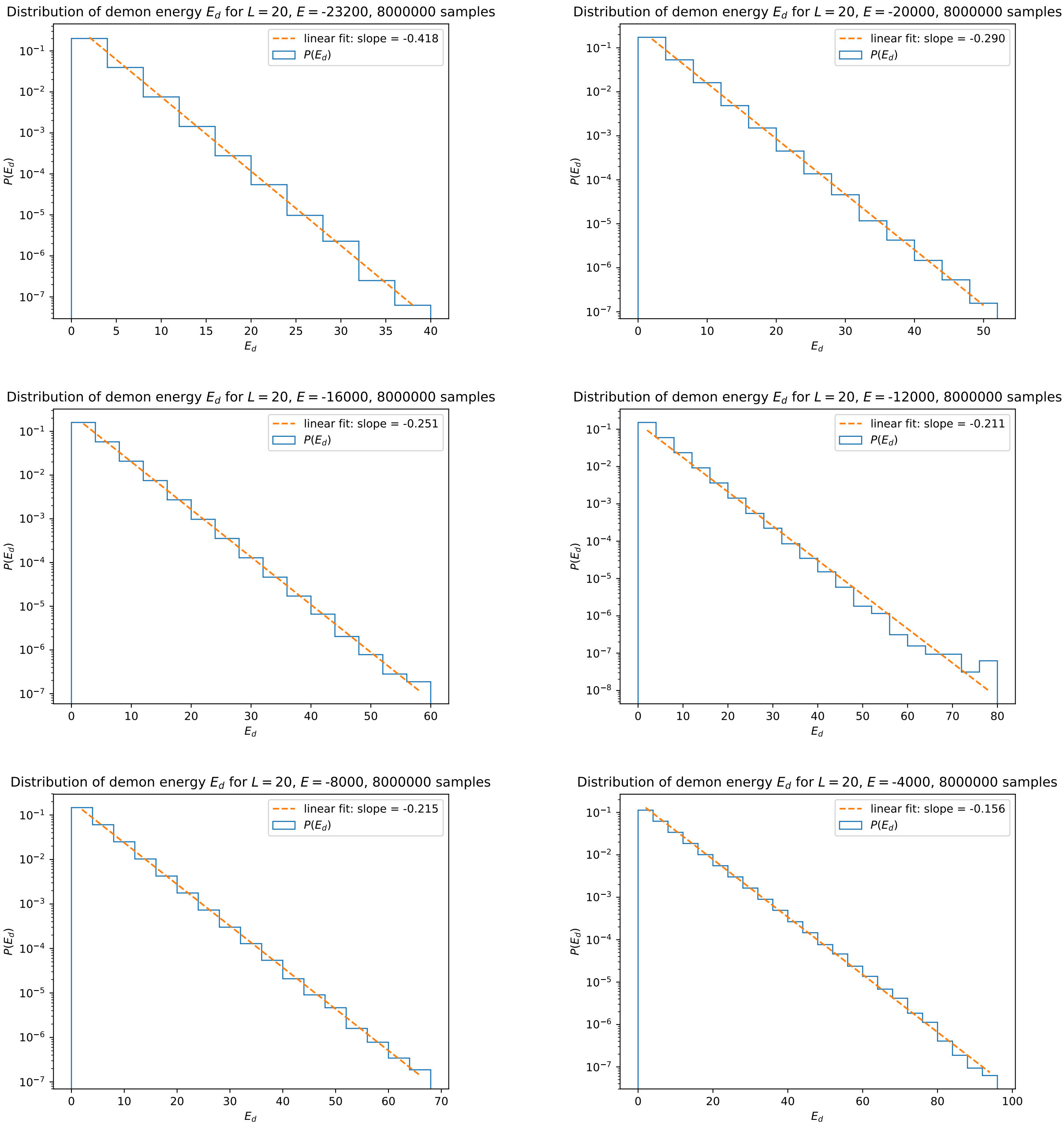

Figure 2: $P(E_d)$ plots for $L = 20$

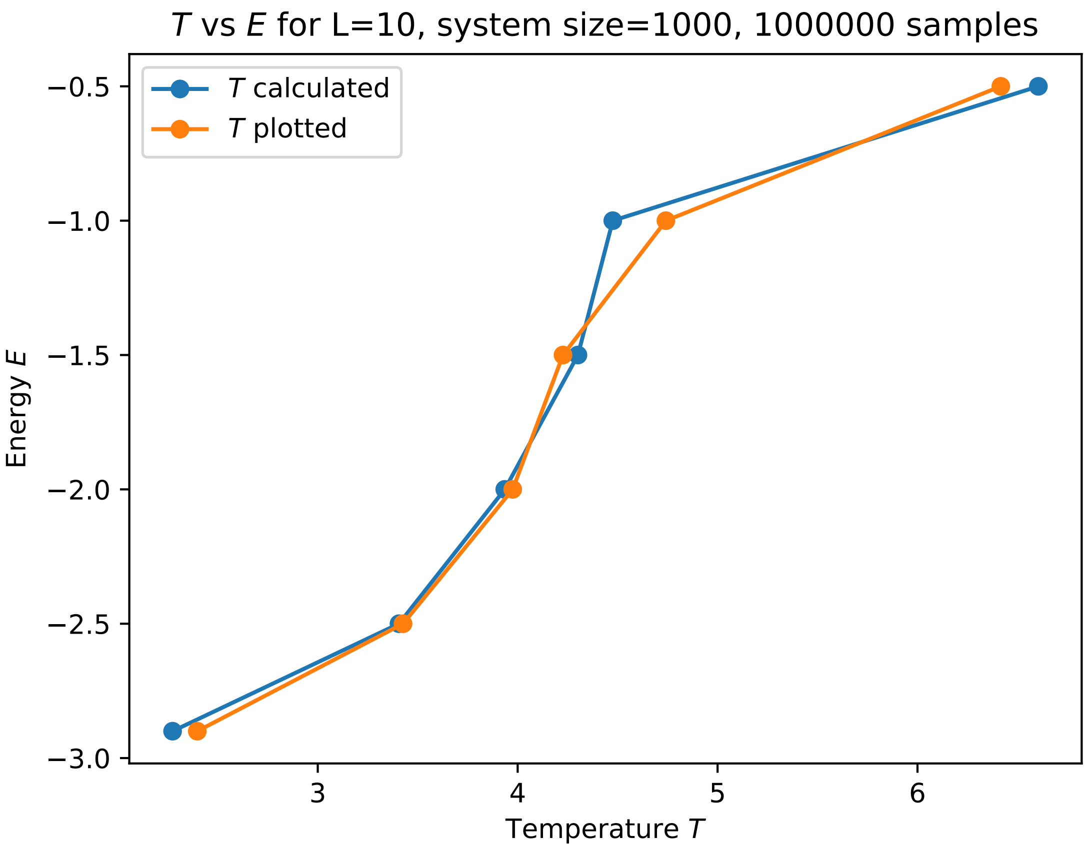

Figure 3: T calculated and plotted versus E for $L = 10$.

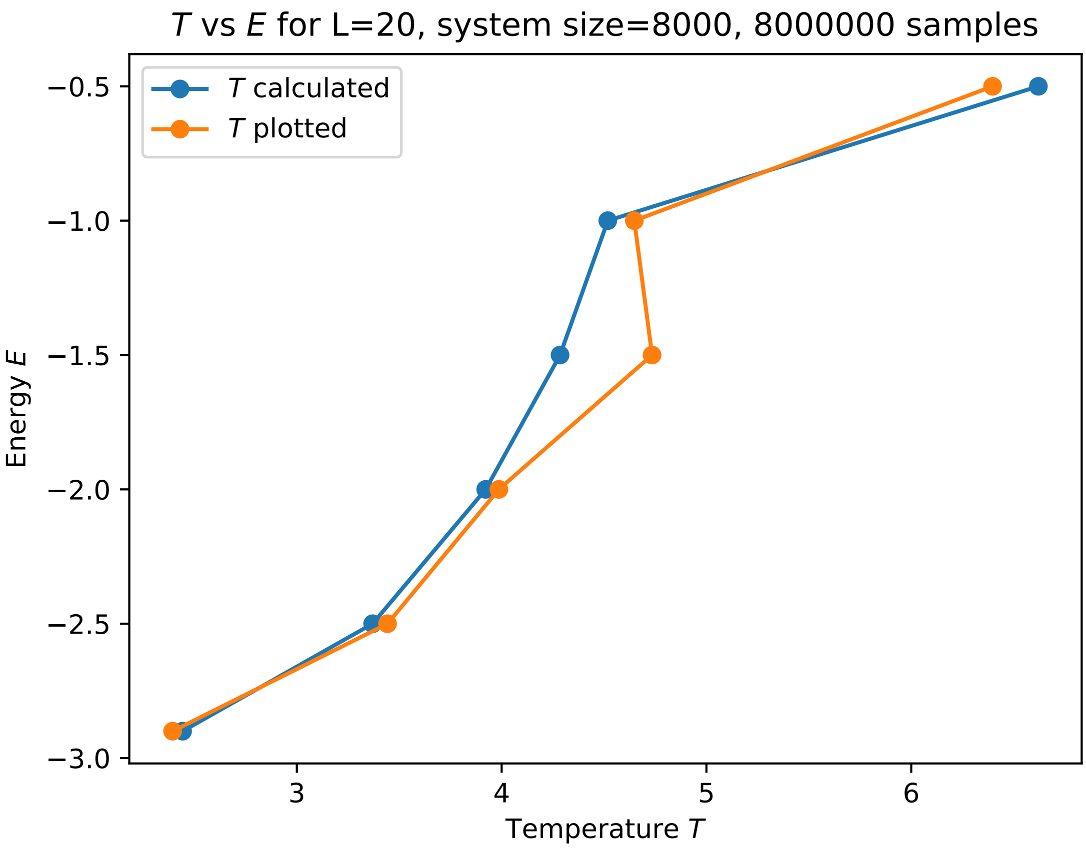

Figure 4: T calculated and plotted versus E for $L = 20$.