Computational Physics - PH3264

Module 2 - Integration

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1. The total magnetic moment of the system is -8000.
2. The total energy of the system is -3000.

Some notes on profiling and performace bottlenecks:

In a Monte Carlo step, the code uses three random numbers to pick a random spin to flip. This computation can be reduced to just one random number. (This is possible thanks to a bijection between the sets $\{0,1,2,3\ldots L^3-1\}$ and $\{(0,0,0),(0,0,1)\ldots(L-1,L-1,L-1)\}$.) The conversion function is given below:

i_to_index(int i) = {i/(L*L), (i/L)%L, i%L}

Profiling with **gprof** (with 50,000 iterations) if three random numbers are generated, the program spends 46.03% of its 2.548 s runtime generating the three numbers. When reduced to one, the program spends only 14.17% of its 1.877 s runtime generating the index, providing a significant performance boost. Additionally, this index conversion is carried out only once per lattice and stored in an array, looked up when required, saving computation time over long cycles.

3. The magnetization per spin of the system fluctuates around 0 - as expected at a higher temperature.

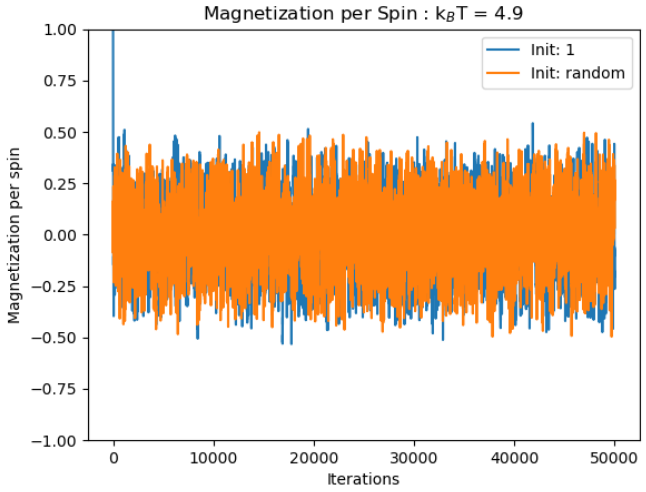

Figure 1: Magnetization per spin at k_BT=4.9

4. The instantaneous energy per spin fluctuates around 2.0 at k_BT=3.9

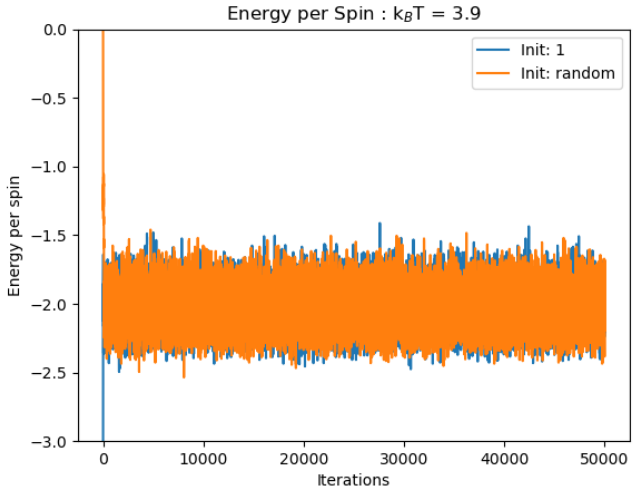

Figure 2: Energy per spin at k_BT=3.9

5. The energy and magnetisation per spin fluctuate about -1.84 and ±0.73 respectively.

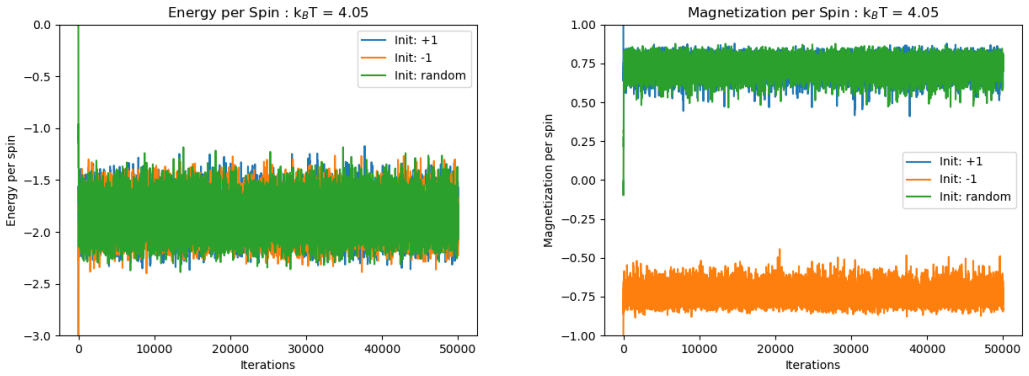

Figure 3: Energy and Magnetization per spin at k_BT=4.05

6. The graphs for Energy and Magnetization at various box sizes have been shown in Figure 4.

The simulation was run as instructed and the following graphs were produced as a result. The magnetisation per spin of the lattice(s) at various temperatures has been plotted in Figure 5. Likewise, the energy per spin can be seen in Figure 6. The plots for χ and C_v are in 7 and 8 respectively.

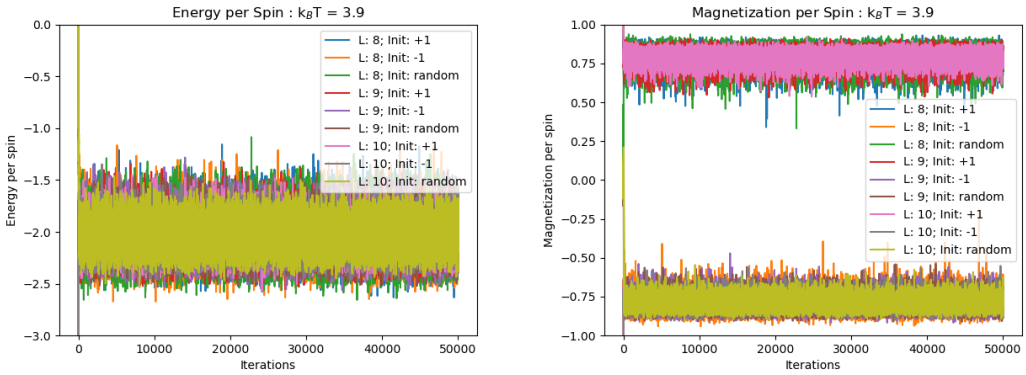

Figure 4: Energy and Magnetization per spin at k_BT=3.9

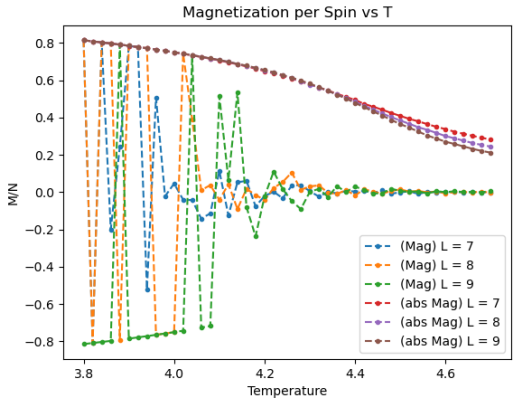

Figure 5: Magnetization per spin vs Temperature

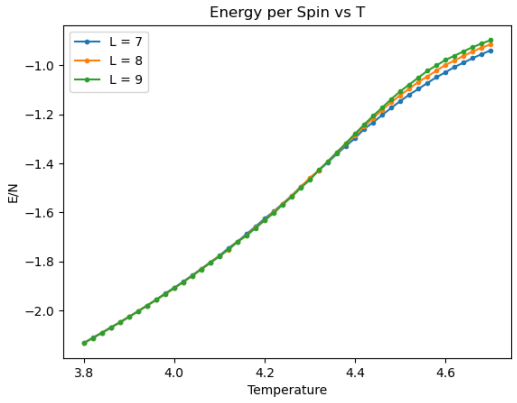

Figure 6: Energy per spin vs Temperature

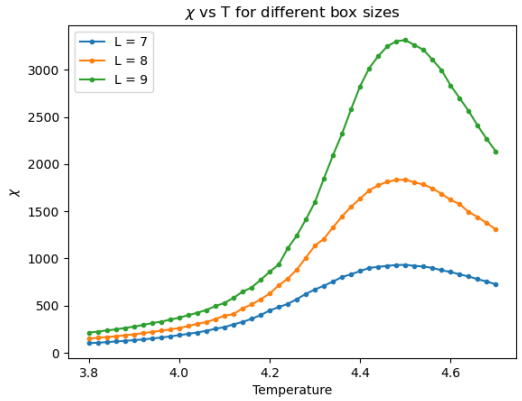

Figure 7: χ vs Temperature

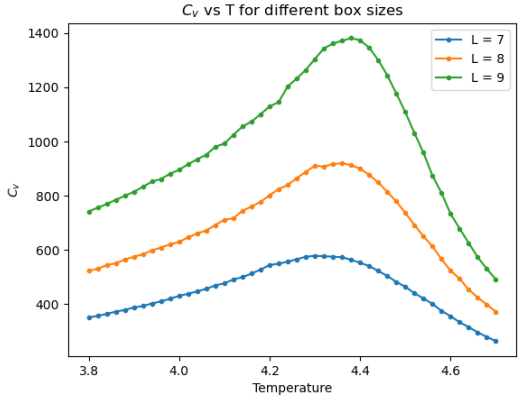

Figure 8: C_v vs Temperature

7. The values of χ at T=4.5 are 932.1, 1835.9 and 3313.7 (in simulation units) for lattice sizes of 7, 8 and 9 respectively.
8. The value fo C_v at peak position for lattice of length 8 is 919.8 (also in simulation units).
9. The value fo C_v at peak position for lattice of length 9 is 1381.7.
10. The magnetization per spin at T = 3.8 for a lattice of length 7 is ± 0.814.
11. The Binder Cumulant plot is shown in Figure 9. The point where the curves intersect is T$\approx$ 4.5.
12. The number of particles jumping from E_{10} to E_5 is $10 \cdot e^{\Delta E \beta}$ where $\Delta E = E_5 - E_{10}$ and $\beta = k_B T$.

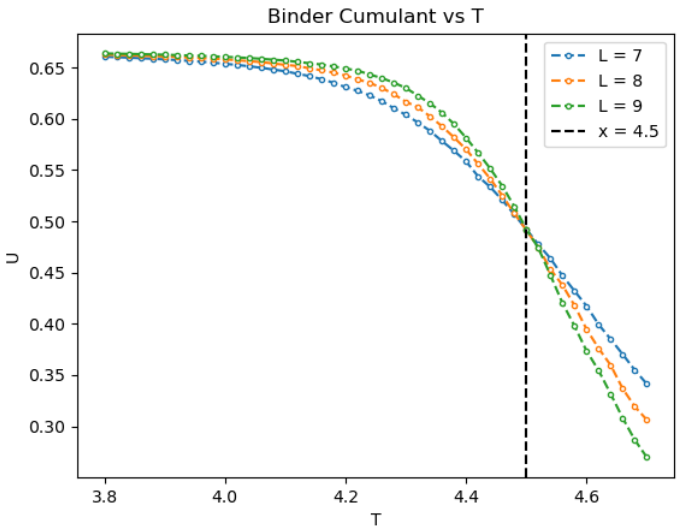

Figure 9: Binder Cumulant for different lattice sizes