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CP III Uebung 8: Metropolis on 3D lattice

In this exercise we should calculate the expectation value of given observables using the Metropolis algorithm. Those values should be calculated for $\lambda = 1.1$ and different κ. Then we should compare those values with a series expansion code given on the course web page. We should find out, for which kappa, then sum is still a good approximation.

In comparison to the last exercise, here we are in a 3D lattice, so we have 16^3 lattice points instead of two. This time we have 6 neighbours insted of 1. The expectationvalue calculated are also different ones, see exercise sheet.

Our Results

Below are printed some results for 10^6 measuring sweeps after 10^5 thermalisation sweeps on a 16^3 lattice. The parameters were $\lambda = 1.1$ and $\kappa = 0.1$.

```
acceptance rate after 1.0e+06 sweeps: 0.551963

A_1:analysing at bin size 10...
value, error and tau_int est. : 0.086571 0.000023 1169403
A_1:analysing at bin size 100...
value, error and tau_int est. : 0.086571 0.000024 1317348
A_1:analysing at bin size 1000...
value, error and tau_int est. : 0.086571 0.000025 1435412
A_1:analysing at bin size 5000...
value, error and tau_int est. : 0.086571 0.000027 1599951
A_1:analysing at bin size 10000...
value, error and tau_int est. : 0.086571 0.000026 1494324

A_2:analysing at bin size 10...
value, error and tau_int est. : 0.769726 0.001830 1411599
A_2:analysing at bin size 100...
value, error and tau_int est. : 0.769726 0.002006 1696694
A_2:analysing at bin size 1000...
value, error and tau_int est. : 0.769726 0.002042 1758566
A_2:analysing at bin size 5000...
value, error and tau_int est. : 0.769726 0.002149 1947515
A_2:analysing at bin size 10000...
value, error and tau_int est. : 0.769726 0.002024 1727588

real    4m46.333s
user    4m46.300s
```

Although the binning error estimate converges as expected, the approximated integrated autocorrelation times τ_{int} seem to be off.

Series Expansion vs. Monte-Carlo Simulation

Here we compare the expectationvalues calculated using metropolis with the expectationvalue using the sum for different values of kappa.

$\kappa = 0.01$

```
Simulation:
acceptance rate after 1.0e+04 sweeps: 0.699786
measured values: A2= 0.564316
Series approximation:
last sum-term 3.72781e-26
A2 = 0.566723
```

$\kappa = 0.05$

```
Simulation:
acceptance rate after 1.0e+04 sweeps: 0.692052
measured values: A2= 0.779794
Series approximation:
last sum-term 3.55512e-12
A2 = 0.767858
```

$\kappa = 0.1$

```
Simulation:
acceptance rate after 1.0e+04 sweeps: 0.672449
measured values:  A2= 1.3062
Series approximation:
last sum-term 3.72781e-06
A2 = 1.31429
```

$\kappa = 0.15$

```
Simulation:
acceptance rate after 1.0e+04 sweeps: 0.642251
measured values:    A2= 3.75251
Series approximation:
last sum-term 0.0123959
A2 = 3.57713
```

$\kappa = 0.2$

```
Simulation:
acceptance rate after 1.0e+04 sweeps: 0.525654
measured values:      A2= 1448.81
Series approximation:
last sum-term 3.9089
A2 = 40.6817
```

From the results above, one can see that the sum is useful up to for the value of $\kappa = 0.15$. For this value, the error is about 5%. One also notices the last sum-term is still very small (10^{-2}). For $\kappa = 0.2$ the results of the sum are useless (the last sum-term ist only one magnitude smaller than the result).