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Computer Simulations in Statistical Physics

Prof. Dr. T. Franosch

Problem set 3

Proseminar

Problem 3.1 *Ising model*

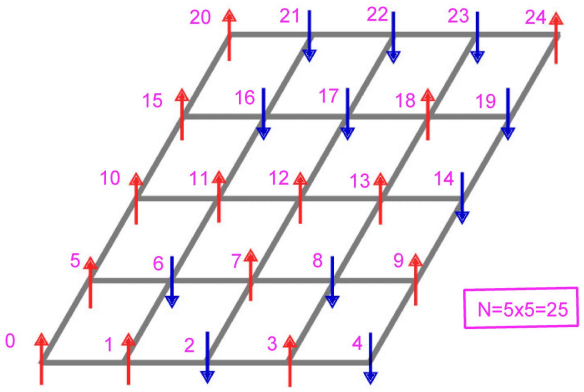
The Ising model is a cornerstone of classical statistical mechanics. It is a mathematical model of ferromagnetism that can be solved exactly in one and two dimensions. In two and higher dimensions the model shows a phase transition.
The Ising model it is defined on a lattice in d dimensions, whose sites are occupied by a spin taking two values $s = \pm 1$. The energy of a configuration $\{s_k\}$ is given by

$$E\left(\{s_k\}\right) = -J \sum_{\langle i,j \rangle} s_i s_j \ , \tag{1}$$

where $J > 0$ is a coupling constant and the sum is extended to nearest neighbors. In the following, we set $J = 1$.

a) Which is the energy of a completely ordered configuration with all spin values equal to 1? What do you expect for the energy of a random configuration?

b) Generate a random configuration of N spins displaced over a square lattice with periodic boundary conditions (take $N = 10 \times 10$) and compute its energy. Programming Hint: think object oriented, i.e. define a class lattice with its own relevant functions. When you add a function to a class, allways test if it is working!
Also remember: it is faster to deal with arrays of size N than with a matrix $\sqrt{N} \times \sqrt{N}$!



c) Repeat the previous point for $M = 100$ different random configurations. Plot the energy E_k with $k = 1, \ldots, M$ and compare the result with the energy of a configuration in which all the spins are equal to 1.

d) use the code snippet "*plot_Ising_configuration.py*" to visualize the configurations.

Problem 3.2 *Ising model - Metropolis algorithm*

We discuss here the Metropolis algorithm for the Ising model. In this algorithm spin configurations are sampled by a Markov chain, which is characterized by a transition probability $P(\mu \to \nu)$ where μ and ν are two spin configurations. In the algorithm $P(\mu \to \nu) \neq 0$ only if the two configurations differ by a single spin. We initialize the system by selecting a random configuration μ of a $N = L \times L$ lattice with periodic boundary conditions. The practical implementation of the algorithm is as follows:

1. Select one of the N spins at random, say spin s_i.
2. Calculate $\Delta E = E_{fin} - E_{in}$, where E_{in} is the energy of the present configuration and E_{fin} the energy of the configuration obtained by flipping the spin $s_i \to -s_i$.
3. Flip the spin $s_i \to -s_i$ if $\Delta E \leq 0$ or if $r \leq \exp(-\Delta E/k_B T)$, where r is a uniform random number in $[0, 1]$.
4. Go to (1).

Typical observables one computes in the Ising model are the energy, as defined by Eq. (1), or the magnetization per spin defined as

$$m = \frac{1}{N} \sum_{i=1}^{N} s_i \ , \tag{2}$$

or spin-spin autocorrelations functions. These quantities reach their equilibrium value after some equilibration time τ_{eq}. Another quantity we compute is the (temporal) autocorrelation function which is defined for a system in which time is a discrete variable

$$\chi(t) = \frac{1}{T} \sum_{s=\tau_{eq}}^{\tau_{eq}+T} \left[m(s) - \langle m \rangle\right] \left[m(s+t) - \langle m \rangle\right] \ , \tag{3}$$

where $m(t)$ is the magnetization at timestep t, and $\langle m \rangle$ is the average equilibrium magnetization. This equation is only valid when the Monte Carlo run has reached an equilibrium configuration ($t > \tau_{eq}$). This autocorrelation function decreases exponentially like

$$\chi(t) \sim \exp\left(-t/\tau\right) \ , \tag{4}$$

where τ defines the autocorrelation time of the simulation. This is the timescale of the simulation, and it indicates how much time it takes to arrive at a new uncorrelated configuration of the model.

a) For a temperature $T = 2$ and $N = 2500$ and starting from a random configuration, use the Metropolis algorithm to compute and plot the energy and the magnetization per spin as a function of the Monte Carlo time step. (For making the plot use the code snippet *"Plot_Ising_trajectory.py"*) Compare the average magnetization with the exact value (valid in the ferromagnetic phase):

$$m(T) = \left[1 - \sinh^{-4}\left(2J/T\right)\right]^{1/8} \ , \tag{5}$$

b) From your plot estimate the equilibration time τ_{eq}.

c) Use the code snippet *"Plot_Ising_trajectory.py"* to visualize time evolution.

d) Determine the correlation time τ (For making the fit and plotting use the code snippet *"Plot_Ising_trajectory.py"*)

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Solution to Problem 3.1 *Ising model*

We start by defining a class "lattice". In this class are contained all relevant functions and subroutines that we can implement on a lattice configurations.

file = lattice.h

```
class Lattice {
  public:
    Lattice(int, double [], double []);      // Constructor
    int get_spin_index(int, int);
    double get_spin_value(double [], int, int);
    int get_right(int);
    int get_left(int);
    int get_above(int);
    int get_below(int);
    double get_energy(double []);

  private:
    int L;
};
```

file = lattice.cpp

```
#include <math.h>
#include "lattice.h"
#include "nrutil.h"

Lattice::Lattice(int N, double s[], double s_initial_values[]){
  // call constructur make a lattice with periodic boundary,
```

```
  // spins initially setted equal to the array "s_initial_values"
  L = sqrt(N);
  for (int i =0; i<N; i++){
    s[i] = s_initial_values[i];
  }
}

int Lattice::get_spin_index(int i, int j){
  // i (j) = row (column) index from 0 to L-1
  // Output: the spin index corresponding to (i,j)
  int k = i*L + j;
  return k;
}

double Lattice::get_spin_value(double s[], int i, int j){
  // i (j) = row (column) index from 0 to L-1
  // Output: the spin value corresponding to (i,j)
  int k = i*L + j;
  return s[k];
}

int Lattice::get_left(int i){
  // return the index of the site at the left of site i
  int j=-1;
  if (i%L == 0){
    j = i+L-1;
  } else {
    j = i-1;
  }
  return j;
}

int Lattice::get_right(int i){
  // return the index of the site at the right of site i
  int j=-1;
  if ((i+1)%L == 0){
    j = i+1-L;
  } else {
    j = i+1;
  }
  return j;
}

int Lattice::get_below(int i){
  // return the index of the site above of site i
  int j=-1;
  if (i<L){
    j = i + (L-1)*L;
  } else {
    j = i-L;
  }
  return j;
}
```

```
60
61
62 int Lattice::get_above(int i){
63   // return the index of the site below of site i
64   int j=-1;
65   if (i>=L*(L-1)){
66     j = (i+L) % (L*L);
67   } else {
68     j = i+L;
69   }
70   return j;
71 }
72
73 double Lattice::get_energy(double s[]){
74   // return the energy E of a given configuration
75   int N = L*L;
76   double E = 0.0;
77   for (int i =0; i<N; i++){
78     E -= s[i]*s[get_right(i)] + s[i]*s[get_below(i)];
79   }
80   return E;
81 }
```

Then we write a very compact "main" file.

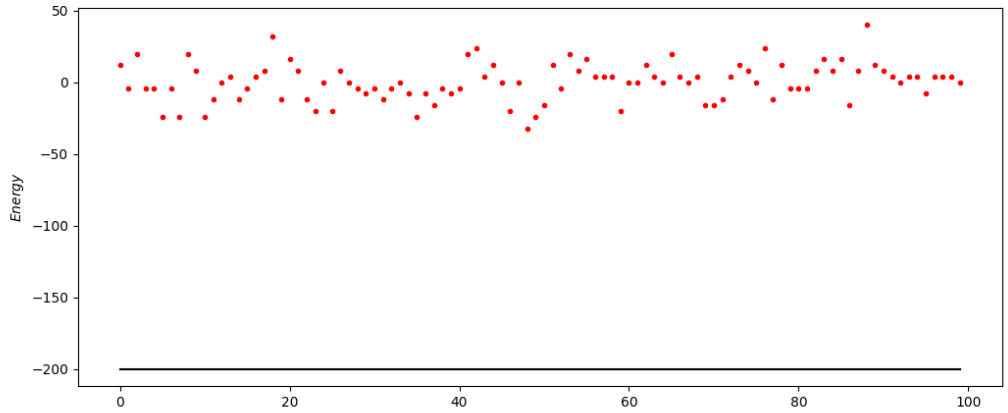
file = Ising.h

```
1  int L;
2  int N;
3
4  double * s;
5  double * s_initial_values;
6  double * s0;
7  double * s1;
8  double * s2;
9  double * s3;
10 double * s4;
11 double * s5;
12
13 double * mvector;
14 double mean (double x[], int NN);
15 double variance (double x[], int NN);
16 double autocorrelation (double x[], int NN, int tau);
```

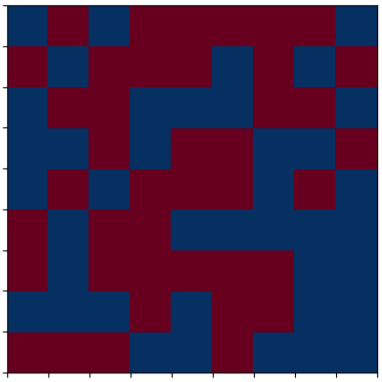
file = Ising.cpp

```
1 // compile with: g++ Ising.cpp lattice.cpp nrutil.cpp -o test -O2 -w
2 #include <stdio.h>
3 #include <stdlib.h>
4 #include <math.h>
5 #include <sstream>
6 #include "Ising.h"
7 #include "lattice.h"
8 #include "nrutil.h"
9
```

```
int main (){
  // set parameters
  L = 10;
  N = L*L;

  // array of length N
  s = dvector(0,N-1);

  // array for a completely ordered configuration
  s_initial_values = dvector(0,N-1);
  for (int i =0; i<N; i++){
     s_initial_values[i] = 1.0;
  }

  /* define lattice as an element of the Lattice class in the
     initial configuration defined by the array "s_initial_values" */
  class Lattice *lattice;
  lattice = new Lattice(N, s, s_initial_values);
  // get the energy of this configuration
  double Energy_order = lattice->get_energy(s);
  printf("%f \n",Energy_order);

  // open output file
  FILE * out;
  out = fopen("output1.dat","w");

  // random configurations
  for (int j=0; j<100; j++){
    for (int i =0; i<N; i++){
      double x = rand()/((double) RAND_MAX)-0.5;
      if (x>0) {
        s[i]=1.0;
      } else {
        s[i]=-1.0;
      }
    }
    double Energy = lattice->get_energy(s);
    fprintf(out,"%d %.4f %.4f \n",j,Energy_order,Energy);
  }
  fclose(out);

  out = fopen("output2.dat","w");
  for (int i =0; i<N; i++){
    fprintf(out,"%.1f \n",s[i]);
  }
  fclose(out);

  return 0;
}
```



Energy of different realizations of random configuration (red points) vs. the energy of a completely ordered configuration (black line).



Visualization of a random configuration.

Solution to Problem 3.2 *Ising model - Metropolis algorithm*

Add the following modules to the lattice class:

file = lattice.cpp

```
double Lattice::get_magnetization(double s[]){
  // return the magnetization m of a given configuration
  int N = L*L;
  double m =0.0;
  for (int i =0; i<N; i++){
    m += s[i];
  }
  m = fabs(m)/N;
  return m;
}
```

```
11
12 void Lattice::Metropolis (double s[], double T, int nmcstep){
13   // perform nmcstep Monte Carlo time steps
14   // using the Metropolis Algorithm
15   // T = temperature
16   int N = L*L;
17   double beta = 1./T;
18   double * precalc;
19   precalc = dvector(-4,4);
20   for (int i=-4; i<=4; i++){
21     precalc[i] = exp(-beta*2*i);
22   }
23   for (int t=0; t<nmcstep; t++){
24     int i = rand() % N;
25     double sum_neigbours = s[get_below(i)] + s[get_above(i)] +
26                            s[get_right(i)] + s[get_left(i)];
27     double E_in = -s[i] * sum_neigbours;
28     double E_fin = s[i] * sum_neigbours;
29     int j = int((E_fin-E_in)/2);
30     if (j<=0) {
31       s[i] = -s[i];
32     } else {
33       if (precalc[j] > rand()/((double) RAND_MAX)) {
34         s[i] = -s[i];
35       }
36     }
37   }
38 }
```

Obviously also the *lattice.h* should be modified accordingly.

And wrap up a main file:

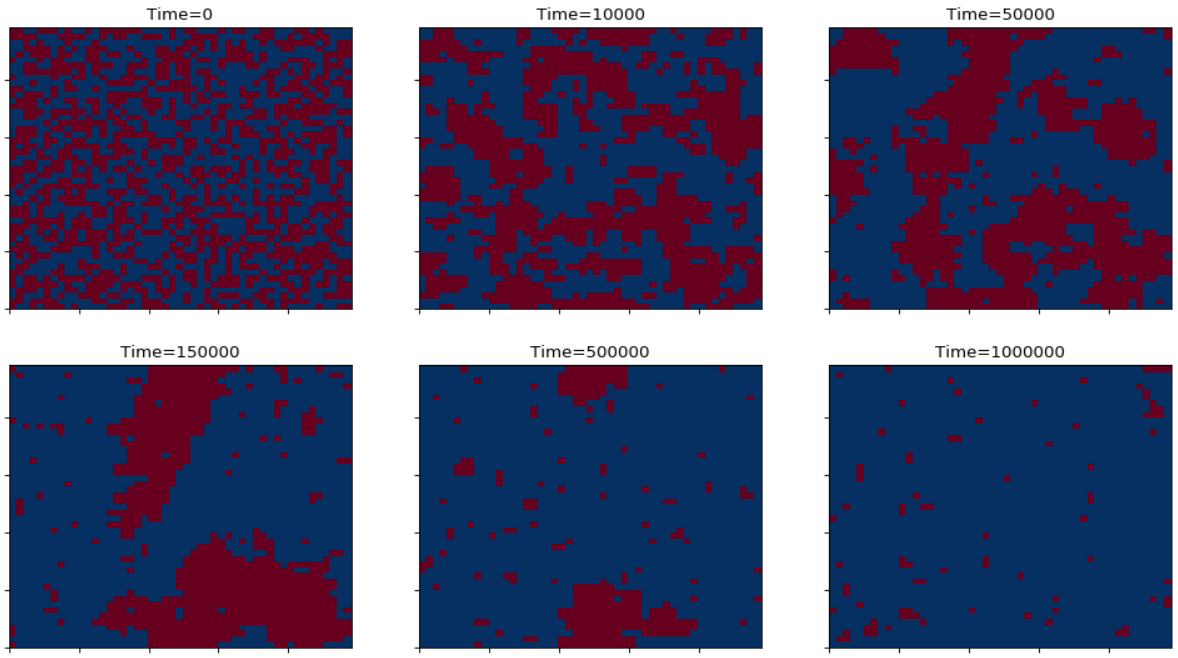
file = Ising_Metropolis.cpp

```
1 // compile with:
2 //   g++ Ising_Metropolis.cpp lattice.cpp nrutil.cpp -o test -O2 -w
3 #include <stdio.h>
4 #include <stdlib.h>
5 #include <math.h>
6 #include <sstream>
7 #include "Ising.h"
8 #include "lattice.h"
9 #include "nrutil.h"
10
11 int main (){
12   // set parameters
13   L = 50;
14   N = L*L;
15   double T = 2.0;
16   int nmcstep = 10000;
17
18   printf("critical temperature = %.4f \n", 2./log(1.+sqrt(2.)));
19   double ma = pow((1.- pow(sinh(2./T),-4.)), 0.125);
```

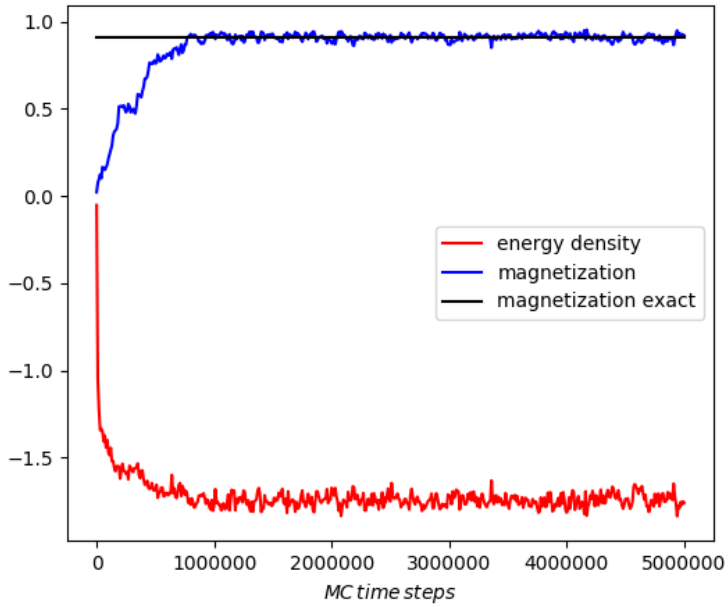
```
20
21    // array of length N
22    s = dvector(0,N-1);
23    s_initial_values = dvector(0,N-1);
24    s0 = dvector(0,N-1);
25    s1 = dvector(0,N-1);
26    s2 = dvector(0,N-1);
27    s3 = dvector(0,N-1);
28    s4 = dvector(0,N-1);
29    s5 = dvector(0,N-1);
30
31    // random configuration
32    for (int i =0; i<N; i++){
33      double x = rand()/((double) RAND_MAX)-0.5;
34      if (x>0) {
35        s_initial_values[i]=1.0;
36      } else {
37        s_initial_values[i]=-1.0;
38      }
39    }
40    class Lattice *lattice;
41    lattice = new Lattice(N, s, s_initial_values);
42
43    // open output file
44    FILE * out;
45    out = fopen("output3.dat","w");
46    double m =  lattice->get_magnetization(s);
47    fprintf(out,"%d %.1f %.4f %.4f \n",0,lattice->get_energy(s), m, ma);
48
49    for (int k =0; k<N; k++) {s0[k]=s[k];}
50
51    // Monte Carlo - Metropolis rule - equilibration
52    int l=0;
53    int j=1;
54    int i=0;
55    while (i<3*j && l==1 || l==0){
56      i++;
57      lattice->Metropolis (s, T, nmcstep);
58      m =  lattice->get_magnetization(s);
59      fprintf(out,"%d %.1f %.4f %.4f \n",
60                           (i+1)*nmcstep,lattice->get_energy(s), m, ma);
61      if (i==1) {
62        for (int k =0; k<N; k++) {s1[k]=s[k];}
63      } else if (i==5) {
64        for (int k =0; k<N; k++) {s2[k]=s[k];}
65      } else if (i==15) {
66        for (int k =0; k<N; k++) {s3[k]=s[k];}
67      } else if (i==50) {
68        for (int k =0; k<N; k++) {s4[k]=s[k];}
69      } else if (i==100) {
70        for (int k =0; k<N; k++) {s5[k]=s[k];}
71      }
72
```

```
    if (m>ma && l==0){
      printf("relaxation time = %d \n", (i+1)*nmcstep);
      j=i;
      l=1;
    }
  }
  fclose(out);

  out = fopen("output4.dat","w");
  for (int i =0; i<N; i++) {
    fprintf(out,"%.1f %.1f %.1f %.1f %.1f %.1f\n",
                        s0[i],s1[i],s2[i],s3[i],s4[i],s5[i]);
  }
  fclose(out);

  // Magnetization autocorrelation function
  //~ nmcstep=1000;
  //~ int nsave = 500000;
  //~ mvector = dvector(0,nsave-1);
  //~ for (int k=0; k<nsave; k++){
    //~ lattice->Metropolis (s, T, nmcstep);
    //~ mvector[k] =  lattice->get_magnetization(s);
  //~ }
  //~ out = fopen("output5.dat","w");
  //~ for (int k =0; k<nsave-10; k++){
    //~ fprintf(out,"%d %f\n",k*nmcstep, autocorrelation (mvector,nsave,k));
  //~ }
  //~ fclose(out);


  return 0;
}

double mean (double x[],int NN){
  // define the mean function
  double xm=0.0;
  for (int i =0; i<NN; i++){
    xm += x[i];
  }
  xm = xm/NN;
  return xm;
}

double variance (double x[],int NN){
  // define the variance function
  double xm=0.0;
  for (int i =0; i<NN; i++){
    xm += x[i]*x[i];
  }
  xm = xm/NN - mean(x,NN)*mean(x,NN);
  return xm;
}

```

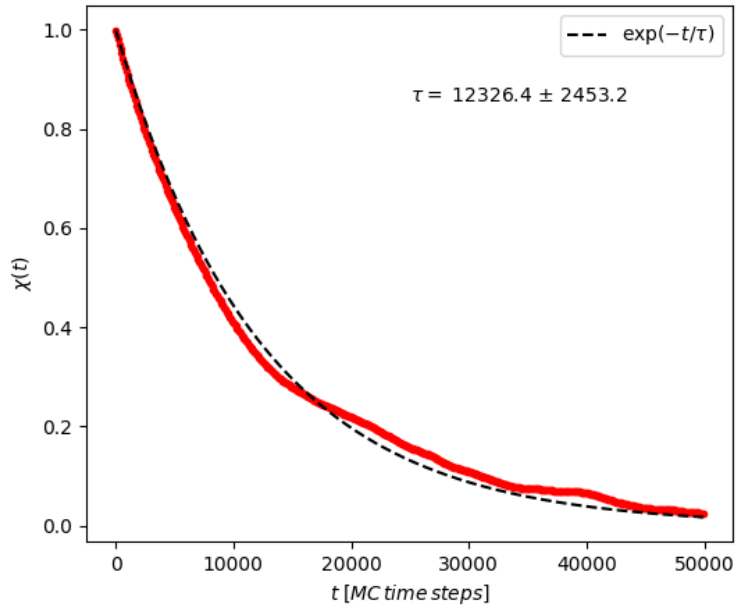
```
126 double autocorrelation (double x[], int NN, int tau){
127   // define the autocorrelation function
128   // input:
129   //   x = 1D array of data
130   //   tau = time lapse
131   // output:
132   //   c_n = autocorrelation of xs at time lapse n
133   double mu1 = mean (x,NN);
134   double sigma2 = variance (x,NN);
135   double c = 0.0;
136   for (int i =0; i<NN-tau; i++){
137     c+=(x[i]-mu1)*(x[i+tau]-mu1);
138   }
139   c = c/(NN-tau);
140   c = c/sigma2;
141   return c;
142 }
```



Visualization of the evolution starting with a random configuration.



Magnetization and energy density as a function of time.



Autocorralation function with a fit to the exponential decay.

Some interesting tricks: A Monte Carlo code consists of a central core nucleus which is repeated a large number of times. Therefore we should try to speed up this core to have a very efficient program (with a fast program we can sample a large number of different configurations

and thus get an accurate result).

- A common mistake is to compute the exponentials at each Metropolis step. The $\exp(x)$ is an operation which requires a certain amount of polynomial approximation on a computer and it is very slow. Since in the Ising model there are only few discrete values for $\Delta E > 0$ (how many?). It is much faster to calculate these once and store these numbers in a small vector.

- To calculate ΔE we only need to know the 4 spins up, down, right and left of the given spin, because all the other spins are unchanged.

- Often one performs simulations at different temperatures, say $T_1 < T_2 < T_3 \ldots$. To avoid long runs to reach equilibration one can take as begin configuration for the simulation at T_2 the last spin configuration of the run at T_1, and so on.