

## Exercises Lecture VIII Ising Model

(results for items in red have to be included in the homework report)

### 1. Ising Model on a square lattice

Write a code for a 2D Ising model on a square lattice in equilibrium with a thermal bath, without external magnetic field, using the **spin flip dynamics** (considered as an actual temporal evolution process), and periodic boundary conditions (PBC). See for instance the code `ising.f90`.

A useful reference paper is D.P. Landau, Phys. Rev. B **13**, 2997 (1976).

Input parameters are:

- L (linear lattice dimension, which gives the number of spins:  $N=L*L$ ),
- *nmcs* (number of total MC steps per spin)
- *nequil* (number of equilibration MC steps per spin)
- T (temperature of the thermal bath).

Quantities of interest are: the *magnetization*:

$$M = \sum_{i=1}^N s_i;$$

the *energy*, with  $\langle i, j \rangle$  all over the nearest neighbor pairs:

$$E = -J \sum_{\langle i, j \rangle} s_i s_j;$$

and quantities related to them, such as the *heat capacity* per spin:

$$c = (\langle E^2 \rangle - \langle E \rangle^2) / k_B T^2 N,$$

and the *magnetic susceptibility* per spin, in absence of an external magnetic field:

$$\chi = (\langle M^2 \rangle - \langle M \rangle^2) / k_B T N.$$

Consider units such that  $k_B=1$ ,  $J=1$ .

- Choose  $L=30$ ,  $T=2$ , and initially spin= $\pm 1$  randomly. Calculate and plot the *instantaneous* values of energy  $\langle E \rangle / N$  and magnetization  $\langle M \rangle / N$  per particle as a function of Metropolis-Monte Carlo steps: how much time (i.e. how many *nequil* MC steps) is necessary to equilibrate the system? Plot the final snapshot of the spin pattern: does the system appear ordered or disordered? Calculate also  $c$  and  $\chi$ .
- Choose  $T=4$  and repeat (a).
- For fixed T, e.g. for  $T=1$  or  $T=2$ , change the initial condition of *magnetization* (choose for instance some typical ordered configurations -all spins up, all spins down, alternatively up or down as on a chessboard, all left hand side spins up and all right hand side down, ...). Does the *equilibration* time change?

- (d) Change the temperature  $T$  by varying it from 1 to 4 with steps of  $\Delta T = 0.5$ . Consider runs long enough, so that the equilibrium has been reached and enough statistical data are collected. Calculate  $\langle E \rangle/N$ ,  $\langle M \rangle/N$ ,  $c$  and  $\chi$ ; plot these quantities as functions of  $T$ . Can you estimate from the plots the *critical temperature* (whose value  $T_c = 2.269 J/k_B$  for 2D is known in case  $L \rightarrow \infty$ )? Calculate numerically  $c$  both in terms of energy fluctuations and doing the numerical derivative with respect to the temperature. Compare the results.
- (e) Repeat now (d) with  $L=4$ . Comment the results.
- (f) Consider the case with *open boundary conditions*. (*Modify the relevant parts of the code concerning the calculation of the energy.*) Repeat some runs with  $L=30$  and  $L=4$ . Comment the results.
- (g) In `ising.f90` the numerical estimate of  $E$  and  $M$  is implemented by *updating E at each MC step over the whole lattice*, i.e. after one (on average) trial move for *all* the spins, chosen randomly one at a time. Choose for instance  $L=30$  and a certain value of  $T$ . Can you see any difference if you choose the spins to flip in an ordered sequence?
- (h) Instead of *updating E* after each MC step over all the spins, do it *for each configuration*, i.e. *after each single MC step per spin*. Compare some results obtained with the two methods, and discuss whether the two methods are equivalent or not.
- (i) (*optional*) It is interesting also to visualise the variation of the spin pattern during the evolution. It can be done using `gnuplot`. (Example available on moodle)

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!cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
!c ising.f90
!c
!c Metropolis algorithm to calculate <E>, <M>, in the canonical ensemble
!c (fix T,N,V) with a 2D Ising model
!c
!c Here: K_B = 1
!c       J   = 1
!c
!cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
module common

  implicit none
  public :: initial,metropolis,DeltaE
  public :: data,output
  integer, public, parameter :: double = selected_real_kind(13)
  real (kind = double), public :: T,E,M
  integer, public, dimension(:,:), allocatable :: spin
  real (kind = double), public, dimension(-8:8) :: w
  integer, public, dimension(4) :: seed      % CHANGE DIMENSION IF NEEDED
  integer, public :: N,L,nmcs,nequil
  integer, public :: accept

```

contains

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subroutine initial(nequil,cum)
  integer, intent (out) :: nequil
  real (kind = double), dimension(5), intent (out) :: cum
  integer :: x,y,up,right,sums,i,dE
  real :: rnd
  print *, "linear dimension of lattice L ="
  read *, L
  allocate(spin(L,L))
  print *, "reduced temperature T ="
  read *, T
  N = L*L
  print *, "# MC steps per spin for equilibrium ="
  read *, nequil
  print *, "# MC steps per spin for averages ="
  read *, nmcs
  print *, "seed (1:4) ="
  read *, seed
  call random_seed(put=seed)
  M = 0.0_double
  ! random initial configuration
  ! compute initial magnetization
  do y = 1,L
    do x = 1,L
      call random_number(rnd)
      if (rnd < 0.5) then
        spin(x,y) = 1
      else
        spin(x,y) = -1
      end if
      M = M + spin(x,y)
    end do
  end do
  ! compute initial energy
  E = 0.0_double
  do y = 1,L
    ! periodic boundary conditions
    if (y == L) then
      up = 1
    else
      up = y + 1
    end if
    do x = 1,L
      if (x == L) then
        right = 1
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        else
            right = x + 1
        end if
        sums = spin(x,up) + spin(right,y)
! calculate the initial energy summing all over pairs
! (for a given spin, consider only the up NN and the right NN
! - NOT the down and the left NN - : each interaction is counted once
        E = E - spin(x,y)*sums
    end do
end do

!
! calculate the transition probability according
! to the Boltzmann distribution (exp(-deltaE/KT).
! Choosing the interaction parameter J=1, ***ONLY IN CASE OF P.B.C.***
! possible energy variations per spin flip are -8,-4,0,+4,+8:
do dE = -8,8,4
    w(dE) = exp(-dE/T)
end do
accept = 0
cum = 0.0_double
end subroutine initial

subroutine metropolis()
! one Monte Carlo step per spin
integer :: ispin,x,y,dE
real :: rnd
do ispin = 1,N
    ! random x and y coordinates for trial spin
    call random_number(rnd)
    x = int(L*rnd) + 1
    call random_number(rnd)
    y = int(L*rnd) + 1
    dE = DeltaE(x,y)
    call random_number(rnd)
    if (rnd <= w(dE)) then
        spin(x,y) = -spin(x,y)
        accept = accept + 1
        M = M + 2*spin(x,y) ! factor 2 is to account for the variation:
        E = E + dE ! ((-)+(+))
    end if
end do
end subroutine metropolis

function DeltaE(x,y) result (DeltaE_result)
! periodic boundary conditions
integer, intent (in) :: x,y

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integer :: DeltaE_result
integer :: left
integer :: right
integer :: up
integer :: down
if (x == 1) then
    left = spin(L,y)
    right = spin(2,y)
else if (x == L) then
    left = spin(L-1,y)
    right = spin(1,y)
else
    left = spin(x-1,y)
    right = spin(x+1,y)
end if
if (y == 1) then
    up = spin(x,2)
    down = spin(x,L)
else if (y == L) then
    up = spin(x,1)
    down = spin(x,L-1)
else
    up = spin(x,y+1)
    down = spin(x,y-1)
end if
DeltaE_result = 2*spin(x,y)*(left + right + up + down)
! also here the factor 2 is to account for the variation
end function DeltaE

subroutine data(cum)
! accumulate data after every Monte Carlo step per spin
real (kind = double), dimension(5), intent (inout) :: cum
cum(1) = cum(1) + E
cum(2) = cum(2) + E*E
cum(3) = cum(3) + M
cum(4) = cum(4) + M*M
cum(5) = cum(5) + abs(M)
end subroutine data

subroutine output(cum)
real (kind = double), dimension(5), intent (inout) :: cum
real (kind = double) :: eave,e2ave,mave,m2ave,abs_mave
real :: acceptance_prob
acceptance_prob = real(accept)/real(N)/real(nmcs+nequil)
eave      = cum(1)/real(N)/real(nmcs)
e2ave     = cum(2)/real(N*N)/real(nmcs)

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    mave      = cum(3)/real(N)/real(nmcs)
    m2ave     = cum(4)/real(N*N)/real(nmcs)
    abs_mave  = cum(5)/real(N)/real(nmcs)
    print *, "temperature          =", T
    print *, "acceptance probability =", acceptance_prob
    print *, "mean energy per spin      =", eave
    print *, "mean squared energy per spin =", e2ave
    print *, "mean magnetization per spin =", mave
    print *, "mean squared magnetization per spin =", m2ave
    print *, "mean |magnetization| per spin =", abs_mave
end subroutine output

end module common

program ising
! metropolis algorithm for the ising model on a square lattice
use common
integer :: imcs,ispin,jspin
real (kind = double), dimension(5) :: cum
call initial(nequil,cum)
! equilibrate system
do imcs = 1,nequil
    call metropolis()
end do
! accumulate data while updating spins
do imcs = 1,nmcs
    call metropolis()
    call data(cum)
end do
call output(cum)

! write the coordinates of spins up and down on files for plotting
open(unit=8,file='ising-up.dat',status='replace')
open(unit=9,file='ising-down.dat',status='replace')
do jspin = 1,L
    do ispin = 1,L
        if (spin(ispin,jspin)==1)write(8,*)ispin,jspin
        if (spin(ispin,jspin)==-1)write(9,*)ispin,jspin
    end do
end do
close(8)
close(9)

deallocate(spin)
end program ising

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