Exercises Lecture IX
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* per spin:

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

   the *energy* per spin, with $< i, j >$ all over the nearest neighbor pairs:

   $$\frac{E}{N} = -\frac{J}{N}\sum_{<i,j>} s_i s_j;$$

   and quantities related to them, such as *time (ensemble) averages*, that we denote with $\langle\rangle$, and response functions, i.e., the *heat capacity* per spin:

   $$c = (< E^2 > - < E >^2)/k_B T^2 N,$$

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

   $$\chi = (< M^2 > - < M >^2)/k_B T N.$$

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

   (a) Choose L=30, T=2, and initially spin=±1 randomly. Calculate and plot the *instantaneous* values of energy E/N and magnetization M/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 χ.

   (b) Choose T=4 and repeat (a).

   (c) 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 χ; 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 $L \to \infty$)? 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)

```
!ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
!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
!ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
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

  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
```

```
    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)
```

```
    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
```