

Exercises Lecture VII 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 $\langle i, j \rangle$ all over the nearest neighbor pairs:

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

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:

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

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 $k_B=1$, $J=1$.

- (a) Choose $L=30$, $T=2$, and initially $\text{spin}=\pm 1$ 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?

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

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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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