

# The Ising model in the canonical ensemble

- Introduction to the Ising model
- The Ising model in the canonical ensemble: application of Metropolis Monte Carlo Method
  - Implementation in a code

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# Spins

Consider two spins  $1/2$ ,  $\vec{s}_1$ ,  $\vec{s}_2$  (e.g. He), their sum  $\vec{S}$ , the basis  $|S, S_z\rangle$  of the Hilbert space in the coupled representation, and a hamiltonian  $\mathcal{H} = h_1 + h_2 + V_{12}$ :

The Pauli principle  $\Rightarrow$  magnetic effects even if  $\mathcal{H}$  does not depend explicitly on spin:

$$\begin{aligned} \langle S = 0 | \mathcal{H} | S = 0 \rangle &= E_s && \text{singlet} \\ \langle S = 1 | \mathcal{H} | S = 1 \rangle &= E_t && \text{triplet} \end{aligned}$$

We have:

$$\langle S = 0 | \mathcal{H} | S = 0 \rangle - \langle S = 1 | \mathcal{H} | S = 1 \rangle = E_s - E_t$$

# Exchange term

**Idea: write a model hamiltonian explicitly dependent on the spin giving the same energy difference between the eigenvalues of its eigenstates as the original one.**

Consider the operator:

$$\Sigma_{12} = \vec{s}_1 \cdot \vec{s}_2 = \frac{1}{2} S^2 - \frac{3}{4}$$

which is diagonal on the coupled base, with eigenvalues:

$$\langle S = 0 | \Sigma_{12} | S = 0 \rangle = -\frac{3}{4}, \quad \langle S = 1 | \Sigma_{12} | S = 1 \rangle = \frac{1}{4}$$

Consider then:

$$\mathcal{H}^{spin} = -(E_s - E_t) \Sigma_{12}$$

We have:

$$\langle S = 0 | \mathcal{H}^{spin} | S = 0 \rangle - \langle S = 1 | \mathcal{H}^{spin} | S = 1 \rangle = E_s - E_t$$

# Heisemberg hamiltonian

$$\mathcal{H}^{spin} = -(E_s - E_t) \Sigma_{12}$$

is therefore OK! Defining:  $J \equiv E_s - E_t$  , we have:

$$\mathcal{H}^{spin} = -J \vec{s}_1 \cdot \vec{s}_2$$

$J > 0$  ( $E_s > E_t$ )     $\uparrow\uparrow$  spins favored => ferromagnetic case

$J < 0$  ( $E_s < E_t$ )     $\uparrow\downarrow$  spins favored => antiferromagnetic case

# Heisemberg hamiltonian

Extension to the case of several spins:

$$\mathcal{H}^{spin} = - \sum_{\substack{i,j=1 \\ i \neq j}}^N J_{ij} \vec{s}_i \cdot \vec{s}_j$$

# Ising model

Consider only the possibility :  $s_i = \pm 1$  and nearest neighbor interaction only, with the same interaction constant  $J$

$$\mathcal{H}^{spin} = -J \sum_{i,j=1}^N s_i s_j$$

- $J > 0$  ( $E_s > E_t$ )     $\uparrow\uparrow$  spins favored => ferromagnetic case  
 $J < 0$  ( $E_s < E_t$ )     $\uparrow\downarrow$  spins favored => antiferromagnetic case

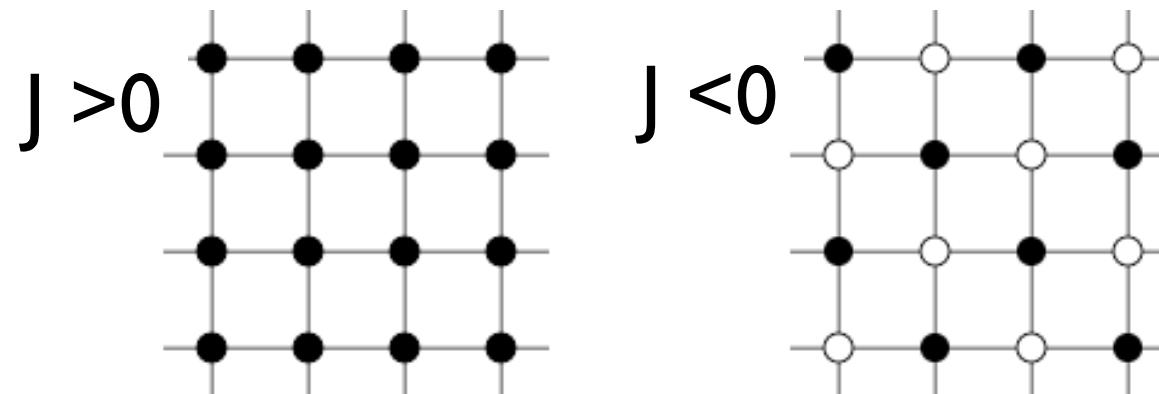


(choosing the kind of interaction, we specify the **energy model**)

# Ising model on a lattice

lattice containing  $N$  sites

lattice site  $i$  has associated with it a number  $s_i$ , where  $s_i = +1$  for an “up” ( $\uparrow$ ) spin and  $s_i = -1$  for a “down” ( $\downarrow$ ) spin. A particular configuration or **microstate** of the lattice is specified by the set of variables  $\{s_1, s_2, \dots, s_N\}$  for all lattice sites.



Lowest energy states of the 2D Ising model on a square lattice with ferromagnetic ( $J>0$ ) and antiferromagnetic ( $J<0$ ) interactions. Solid and open circles correspond to  $+1$  and  $-1$  spins, respectively.

# Ising model: interesting quantities

# Ising model: energy

lattice containing  $N$  sites

No external magnetic field:

$$E = -J \sum_{i,j=\text{nn}(i)}^N s_i s_j$$

(nn=nearest neighbor)

Energy in presence of an external magnetic field:

$$E = -J \sum_{i,j=\text{nn}(i)}^N s_i s_j - H \sum_{i=1}^N s_i,$$

or, better, define an **average energy per spin**:  $E/N$

# Ising model: magnetization

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

Total magnetization, or define an average magnetization per spin:

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

$$-1 \leq m \leq +1$$

# Ising model: configurations and energy

$2^n$  different configurations for  $n$  spins.

e.g.  $2^4 = 16$  spin configurations for  $2 \times 2$  lattice

$$\begin{array}{cc} + + & - - \\ + + & - - \end{array} \quad \begin{array}{cc} + - & - + \\ - + & + - \end{array}$$

$$\begin{array}{cccccccccccccccc} - + & + - & + + & + + & + - & - + & - - & - - & - - & + - & + + & - + \\ + + & + + & + - & - + & - - & - - & - + & + - & + + & + - & - - & - + \end{array}$$

---

For  $J > 0$  the state of lowest energy is when all the spins are aligned.  
The state has macroscopic magnetization (**ferromagnetic**).

The **ground state energy** per spin

(ferromagnetic case, thermodynamic limit ( $N$  large), no ext. field) is:

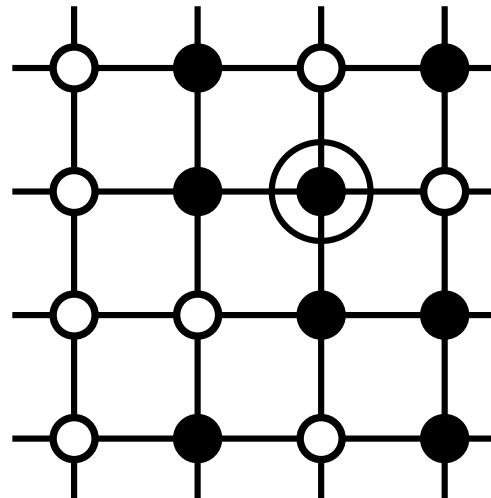
$$E_0/N = - 2J$$

# Ising model: dynamics?

Beside an **energy model**, we must define a **dynamics** in order to simulate the evolution of the system (i.e. to generate the trajectory in the phase space, to generate the configurations of the Markov chain)

# Ising model: spin flip dynamics

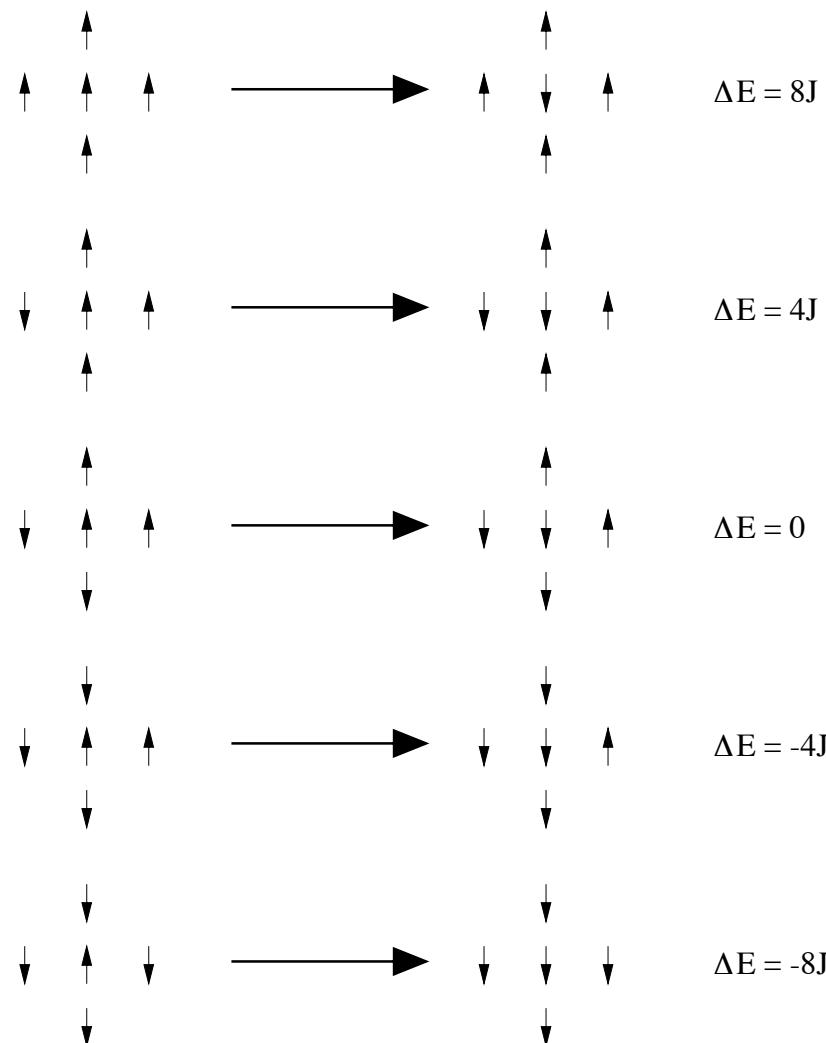
Consider  $nn$  interactions, choose a random spin and flip it: it's a **new configuration** (a microstate)



Apply **Metropolis Monte Carlo** method for evolution in the **canonical ensemble** (fix  $T$ ). Evolution is driven by the **energy change** between the old and the new configuration,  $\Delta E$ .

**Remark:** Is it sufficient to calculate only  $\Delta E$ , not  $E$  at each new configuration!

# Ising model: spin flip dynamics



The five possible transitions of the Ising model on the square lattice with spin flip

# Ising model: boundary conditions

Of course we cannot simulate an infinite system  
(the thermodynamic limit).

We have two choices for the simulation cell:

- free (open) boundary conditions
- periodic boundary conditions (PBC)

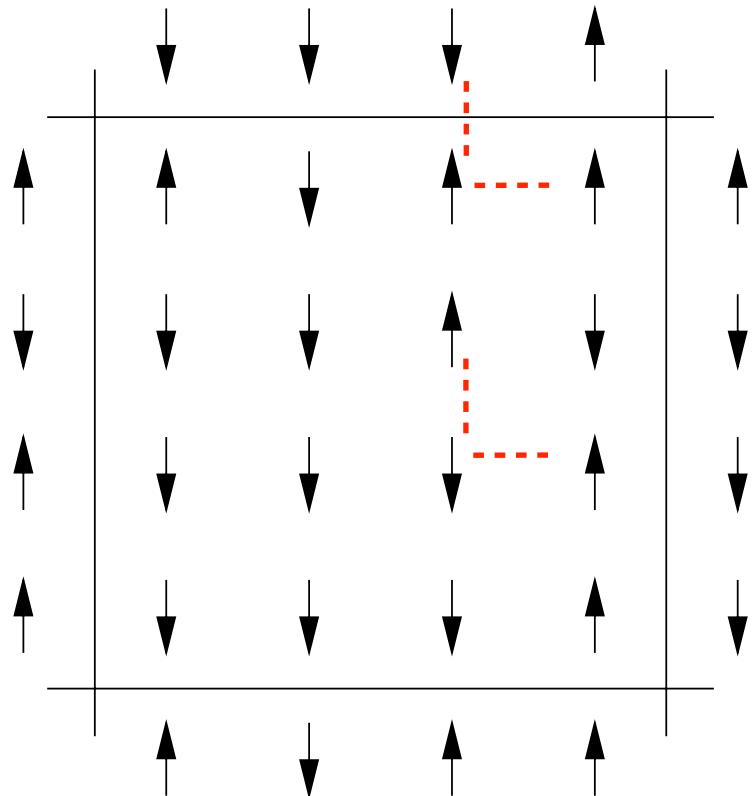
# Ising model: free boundary conditions

in a  $N=L \times L$  spin lattice there are  $2L(L-1)$  nn interactions; for the ferromagnetic g.s. configuration, for instance, the energy is:

+	+	+	+	
+	+	+	+	
+	+	+	+	
+	+	+	+	
E <sub>0</sub> /N = -J	E <sub>0</sub> /N = -(12/9)J	E <sub>0</sub> /N = -(24/16)J	...	E <sub>0</sub> /N = -J × 2L(L-1)/L <sup>2</sup> = -2J × (1-1/L)
				(volume term)      (surface term)

Energy per spin in the ground state converges to the value  
 $E_0/N = -2J$  in the thermodynamic limit  
as  $1/L$  in case of free boundaries

# Ising model: PBC



The energy is a  $2N$ -term sum:  
each spin interacts with its NN  
within the simulation cell or  
with the NN images

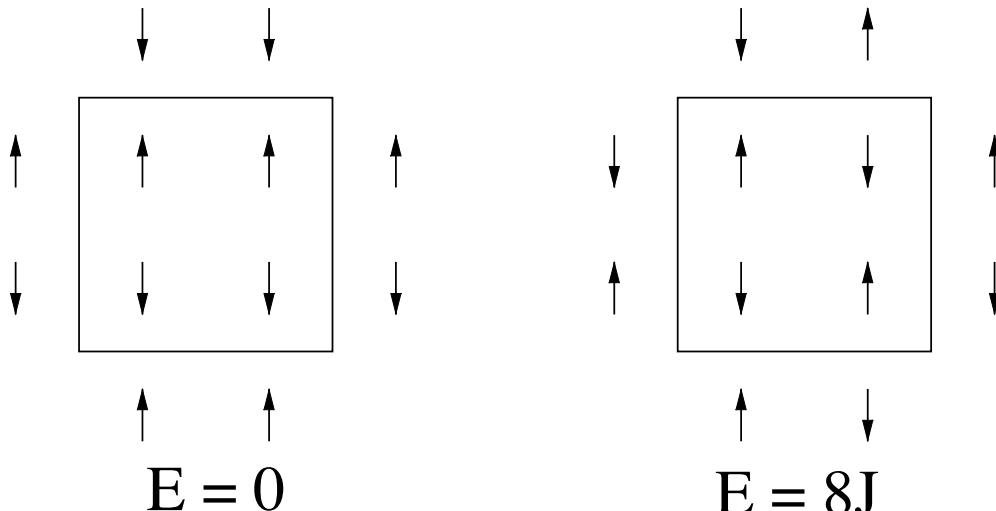
One of the  $2^N$  possible configurations of a system of  $N = 16$  Ising spins on a square lattice.  
with periodic boundary conditions.

# Ising model: PBC

We have always:

$$2^4 = 16 \text{ spin configurations for } 2 \times 2 \text{ lattice}$$

but the energy for each configuration in case of free boundary conditions and PBC is different:



Two different configurations with 2 spins up

# of spins UP	Degeneracy	Energy	Magnetisation
4	1	$-8J$	4
3	4	0	2
2	4	0	0
2	2	$8J$	0
1	4	0	-2
0	1	$-8J$	-4

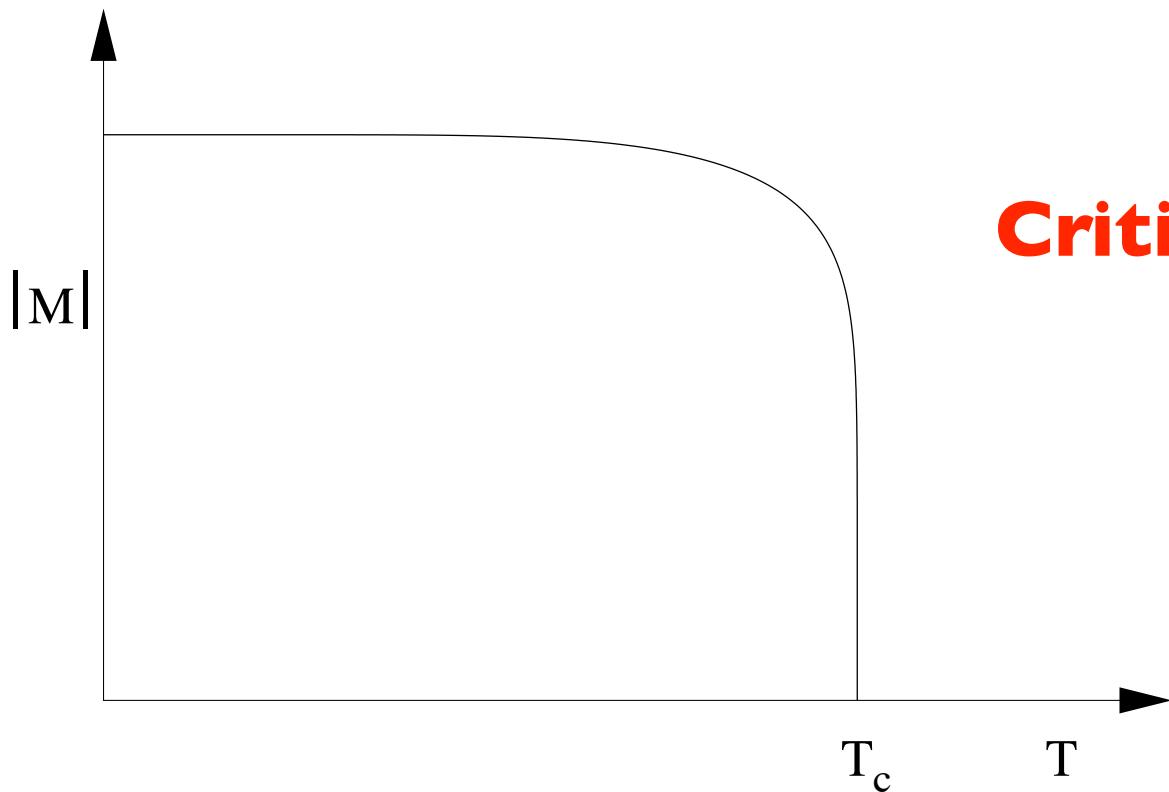
Energy and magnetization of 16 configurations of the  $2 \times 2$  Ising model with PBC

Energy per spin in the ground state is always equal to the value  $E_0/N = -2J$  in the thermodynamic limit

# Ising model: phase transition

**Low T: spin configuration minimizes energy**  
(if  $J > 0$ : spins tend to align => **high (absolute) magnetization**)

**High T: spin configuration maximizes entropy**  
**(=disorder)** (spins tend to disalign => **low magnetization**)

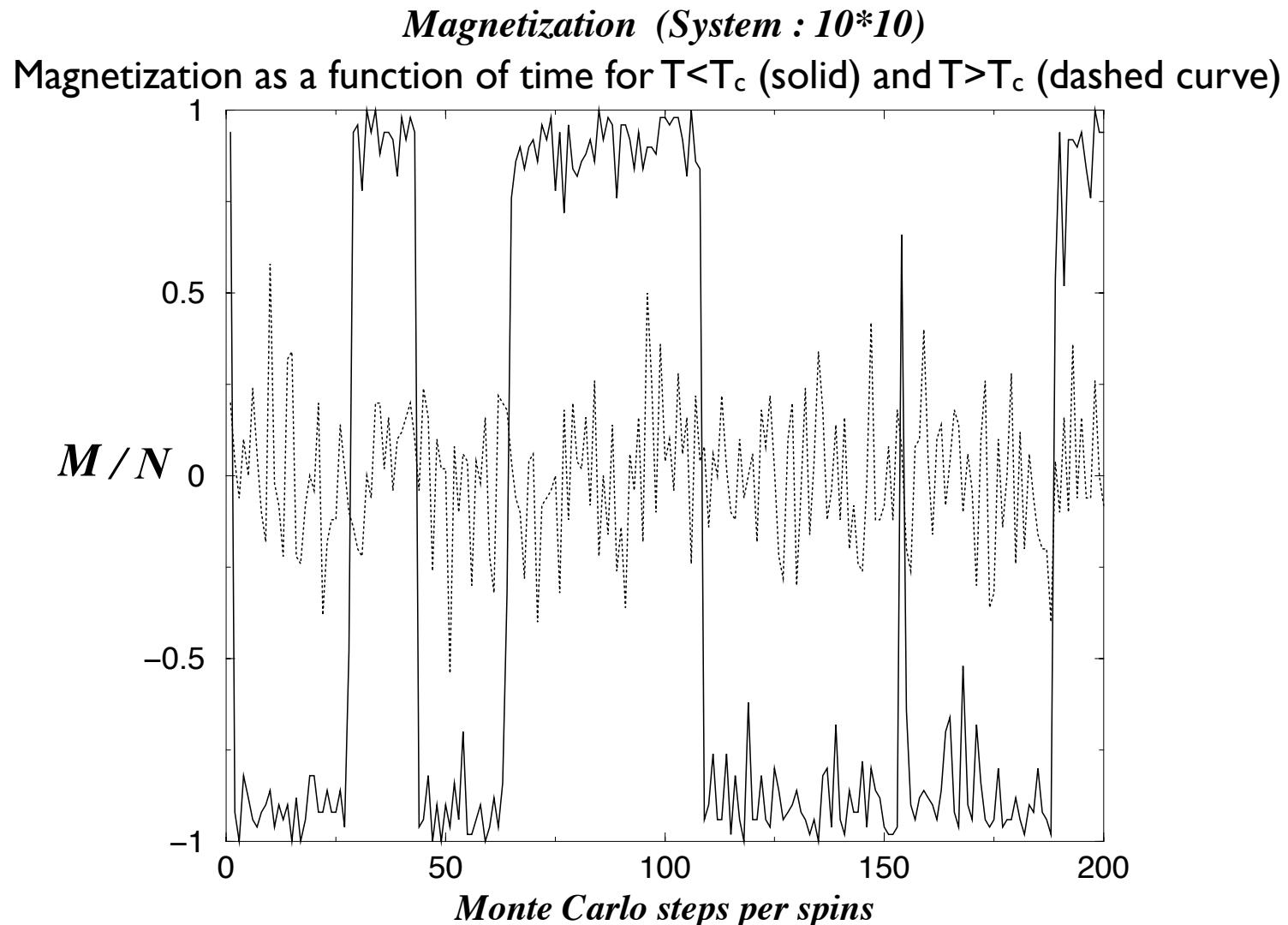


**existence of a  
Critical temperature  $T_c$**

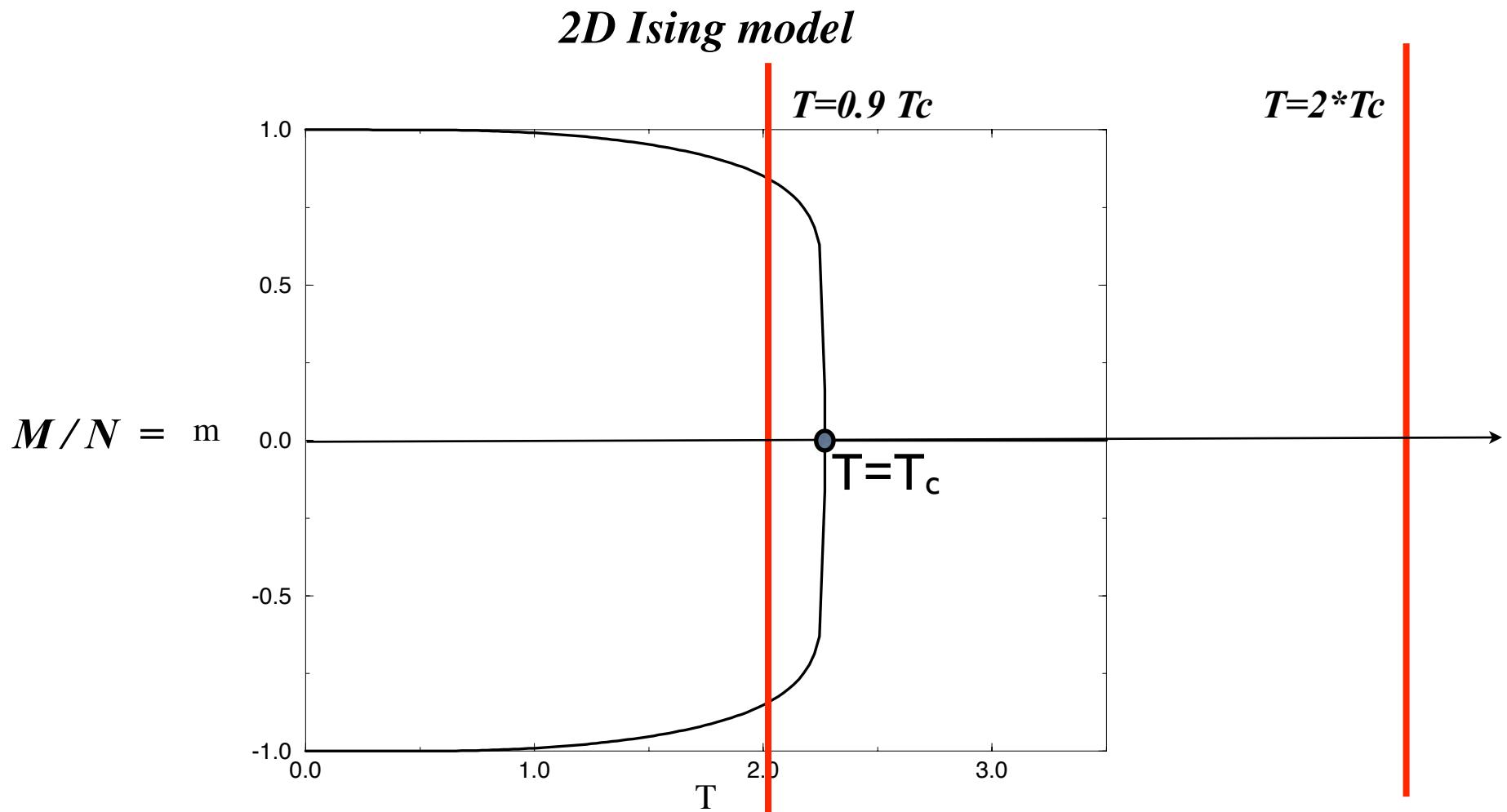
in 2D:

$$T_c = 2.269 \text{ J}/k_B$$

Apply **Metropolis Monte Carlo** method for evolution in the **canonical ensemble** (fix T):

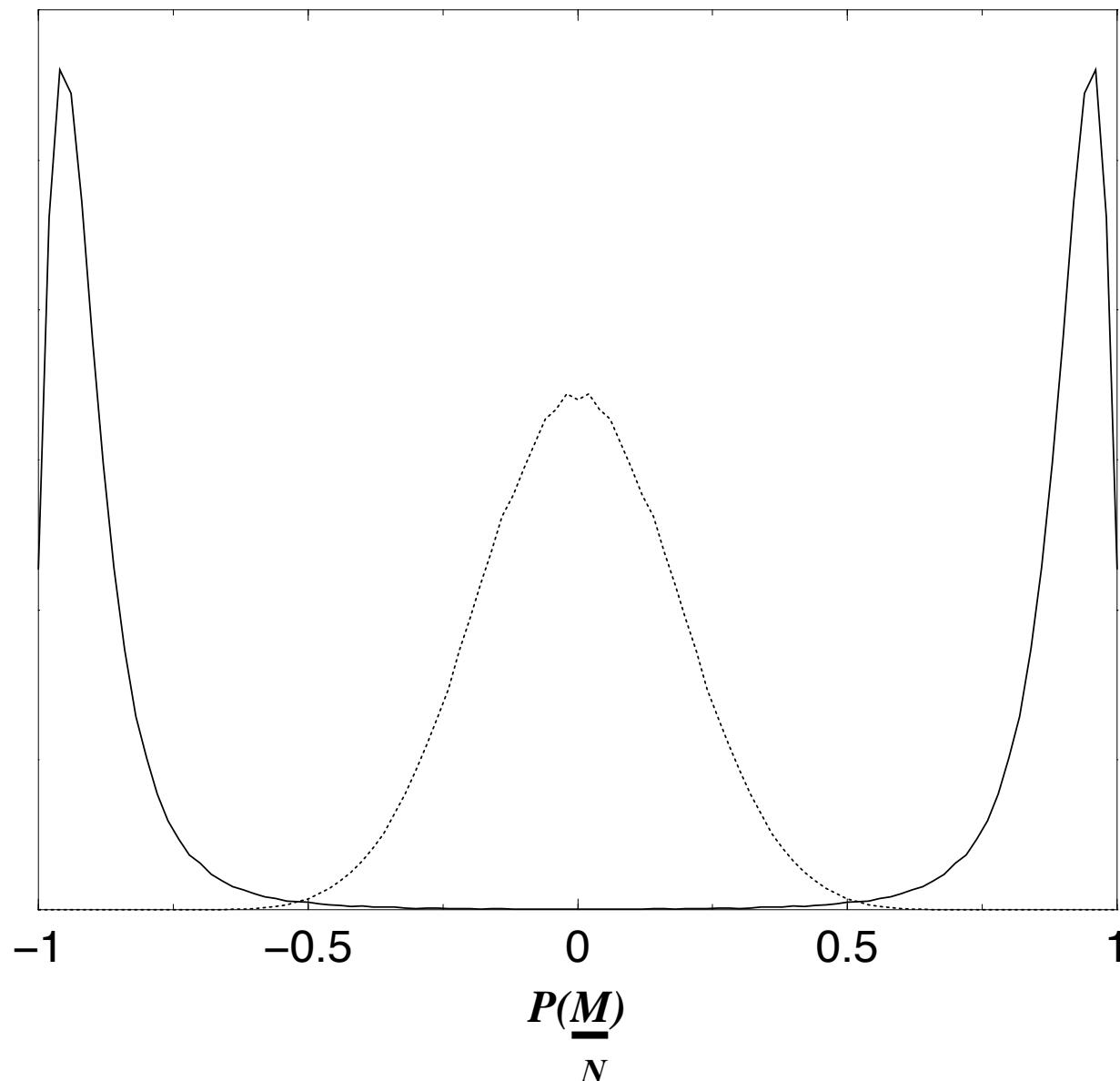


Fluctuations! do, as usual, **temporal averages**:  $\langle M/N \rangle$ ,  $\langle E/N \rangle$



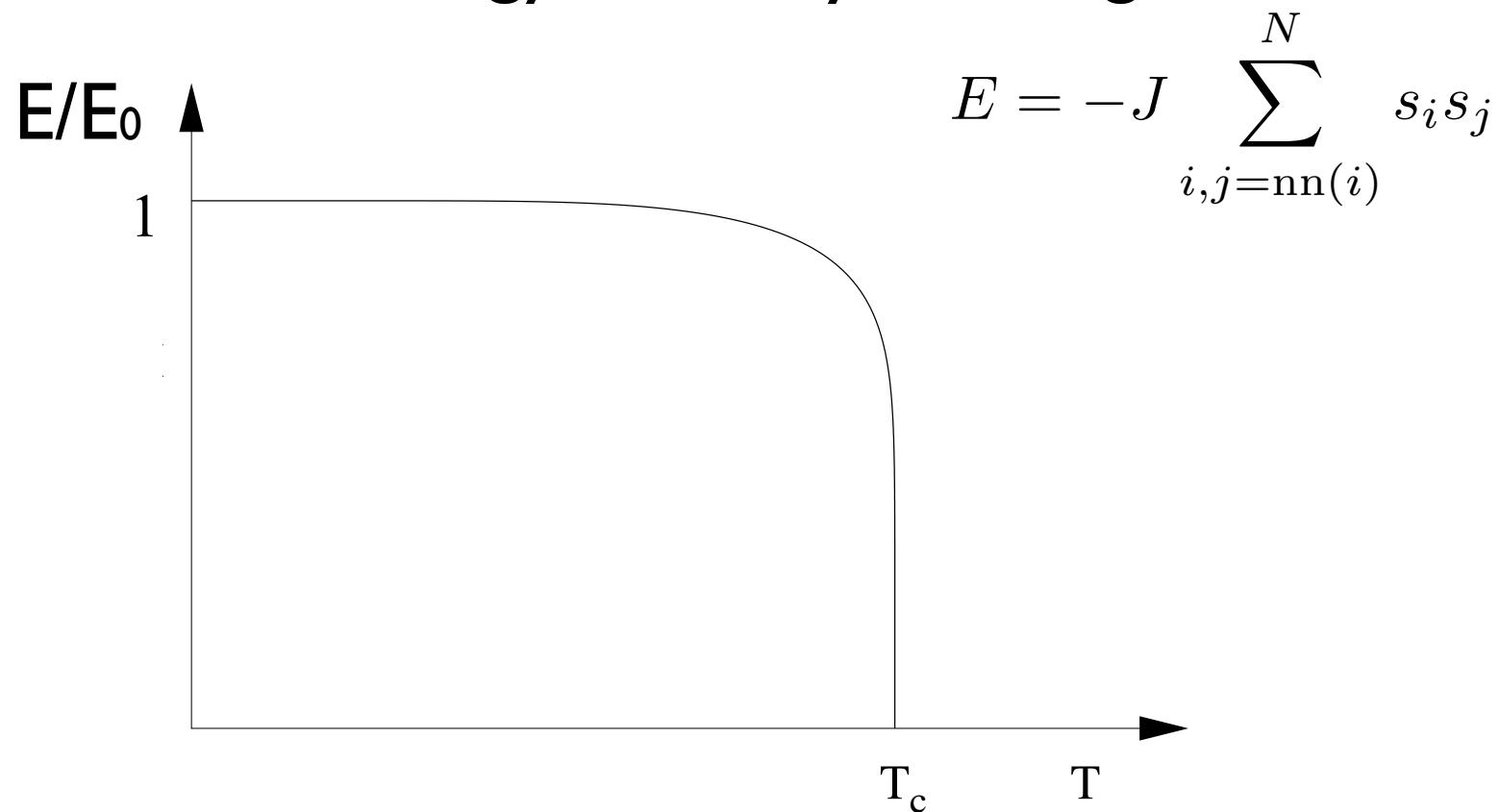
Magnetisation as a function of the temperature for the 2D Ising model.

## Magnetization distribution for $T < T_c$ (solid) and $T > T_c$ (dashed curve)



# Ising model: phase transition

$T_c$  also for energy, not only for magnetization:



and also the energy fluctuates during time evolution...

# Ising model: fluctuations

Fluctuations are intrinsic to the system evolution  
and are important!

Linear response functions are related to  
equilibrium fluctuations:

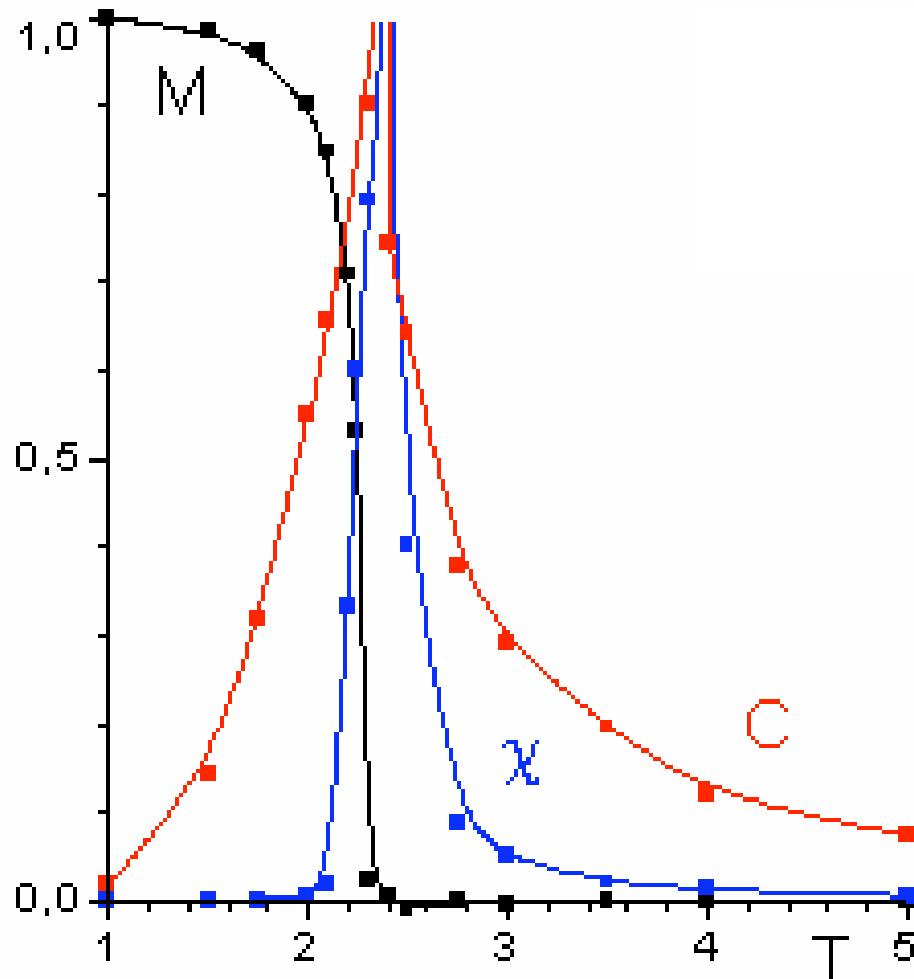
(already proved):  $C = \frac{\partial \langle E \rangle}{\partial T}$ ,  $C = \frac{1}{kT^2} (\langle E^2 \rangle - \langle E \rangle^2)$

but also:  $\chi = \lim_{H \rightarrow 0} \frac{\partial \langle M \rangle}{\partial H}$ ,  $\chi = \frac{1}{kT} (\langle M^2 \rangle - \langle M \rangle^2)$

where  $\langle M \rangle$  and  $\langle M^2 \rangle$  are evaluated in zero magnetic fields.

# Ising model: fluctuations and phase transition

Rapid change in  $\langle E \rangle$  and  $\langle M \rangle \Rightarrow$  singularities in  $C$  and  $\chi$



(Large fluctuations near  
the phase transition:  
Second Order phase transition)

specific heat:

$$C = \frac{\partial \langle E \rangle}{\partial T}$$

magnetic susceptibility:

$$\chi = \lim_{H \rightarrow 0} \frac{\partial \langle M \rangle}{\partial H}$$

# Implementing the Ising model in the code

# Implementing the Ising model

on a 2D square lattice in the canonical ensemble  
zero-field, nearest neighbor interactions only

$$\mathcal{H}^{spin} = -J \sum_{i,j=1}^N s_i s_j \quad s_i = \pm 1$$

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).

# Implementing the Ising model

```
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)
.....
.....
end program ising
```

# Ising model on a lattice

L : linear lattice dimension

N = LxL : number of spins

a **configuration** (a microstate) is the whole sequence of spins, i.e. the LxL array spin(x,y)

module common

.....

```
integer, public, dimension(: ,:), allocatable :: spin
```

```
subroutine initial(nequil,cum)
```

.....

```
allocate(spin(L,L))
```

.....

```
    spin(x,y) = 1
```

```
else
```

```
    spin(x,y) = -1
```

.....

$$s_i = \pm 1$$



# Ising model: magnetization

Total magnetization, or define an average magnetization per spin:

```
! compute initial magnetization
M = 0.0_double
do y = 1,L
  do x = 1,L
    ....
    ....
    M = M + spin(x,y)
  end do
end do
```

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

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

$$-1 \leq m \leq +1$$

(Instead of the loop over x,y, do also simply: `M=sum( spin )` )

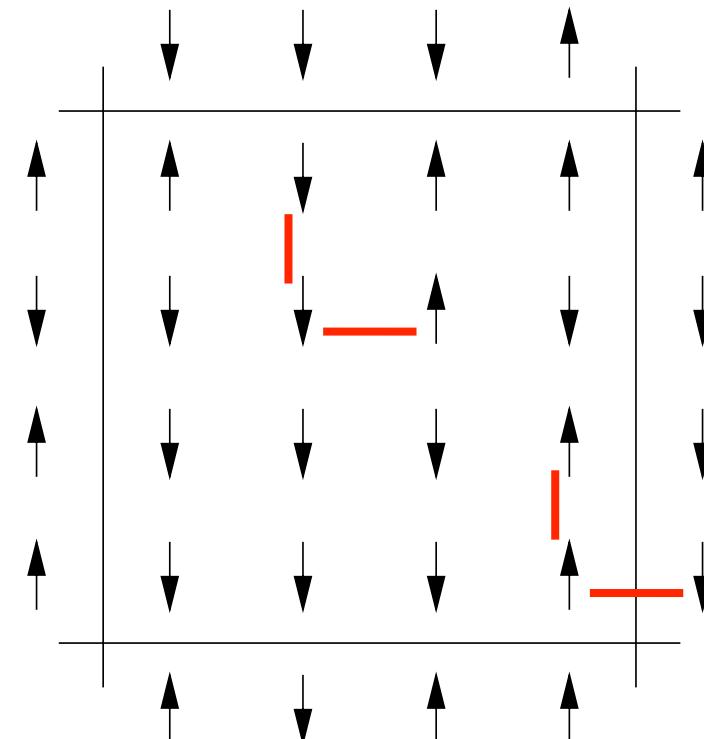
# Ising model: energy

$$E = -J \sum_{i,j=\text{nn}(i)}^N s_i s_j$$

```
!  compute initial energy
E = 0.0_double
do y = 1,L
.....
  do x = 1,L
    .....
      sums = spin(x,up) + spin(right,y)
      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
```

# Ising model: energy with PBC

```
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
        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
```



# Ising model: spin flip dynamics

Choose a random spin and flip it:  
**it's a new configuration** (a microstate)

```
do ispin = 1,N
    !      random x and y coordinates for trial spin
    call random_number(rnd)
    x = int(L*rnd) + 1           ← 1 ≤ x ≤ L
    call random_number(rnd)
    y = int(L*rnd) + 1           ← 1 ≤ y ≤ L
    ....
```

Flip is:  $\text{spin}(x,y) = -\text{spin}(x,y)$

but do it later, only if you decide to accept the flip (according to Metropolis)

# Ising model: energy variations per spin flip

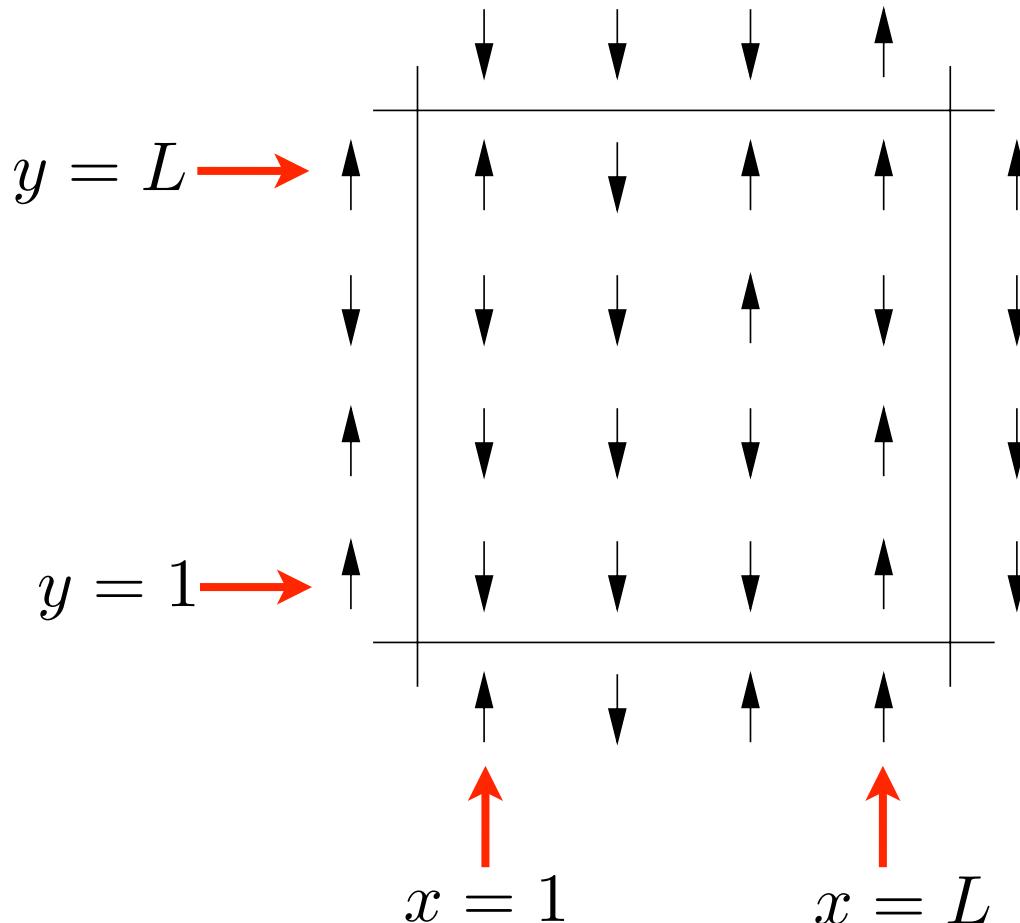
Evolution is driven by the **energy change** between the old and the new configuration (Metropolis MC)

```
dE = DeltaE(x,y) ← energy variation for spin(x,y) flip  
call random_number(rnd)  
if (rnd <= w(dE)) then ← w(dE) is  $e^{-\Delta E/k_B T}$   
    spin(x,y) = -spin(x,y)  
    accept = accept + 1  
....  
....
```

```
function DeltaE(x,y) result (DeltaE_result)  
....  
DeltaE_result = 2*spin(x,y)*(left + right + up + down)  
....
```

# Energy variations per spin flip with PBC

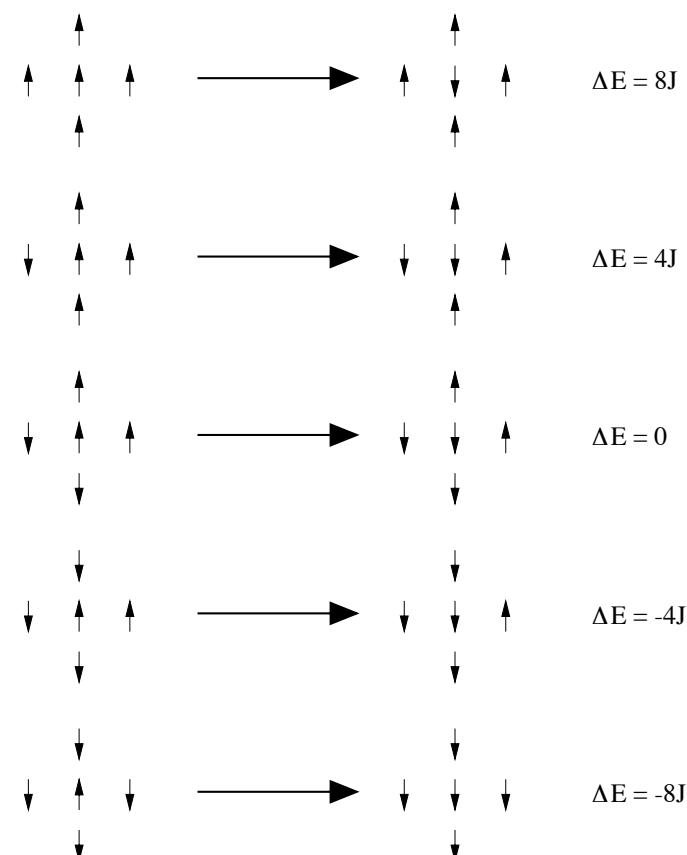
```
function DeltaE(x,y) result (DeltaE_result)
    ! periodic boundary conditions
.....
if (x == 1) then
    left = spin(L,y)
    right = spin(2,y)
else if (x == L) then
    left = spin(L-1,y)
    right = spin(1,y)
else
    left = spin(x-1,y)
    right = spin(x+1,y)
end if
if (y == 1) then
    up = 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)
.....
```



# Ising model: storage of Boltzmann's coeff.

! Choosing the interaction parameter  $J=1$ ,  
! 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  
do i = 1,5  
    cum(i) = 0.0_double  
end do
```



Convenient to store the Boltzmann's coefficient for these discrete values of energy variations

The five possible transitions of the Ising model on the square lattice with spin flip

# Ising model: updating energy and magnetization

```
subroutine metropolis()
    ! one Monte Carlo step per spin
    .....
    .....
    do ispin = 1,N
    .....
        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
```

DO NOT CALCULATE  
EVERYTHING FROM THE  
SCRATCH!!

$\Delta E$  is already a variation

# Spin flip dynamics: how to choose spin to flip?

Random ...

```
do ispin = 1,N
    !      random x and y coordinates for trial spin
call random_number(rnd)
x = int(L*rnd) + 1           ← 1 ≤ x ≤ L
call random_number(rnd)
y = int(L*rnd) + 1           ← 1 ≤ y ≤ L
....
```

or ordered (sequential) ...

```
do x = 1,L
do y = 1,L
...
spin(x,y) = -spin(x,y)
```

# Spin flip dynamics: how to choose spin to flip?

- ORDERED: in some cases, it could go more slowly towards equilibrium (see later: correlation time), but it depends...
- NO appreciable differences in the statistics at equilibrium

# Measuring physical quantities: how to accumulate data?

```
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
```

After one MC step per spin for all spins:

```
do imcs = 1,nmcs
  call metropolis()           contains the loop over all the spins
  call data(cum)
end do
```

Alternatively, do it after each MC step per individual spin...

# Measuring physical quantities: how to accumulate data?

## Further remarks...

- Use statistically **INDEPENDENT** configurations
- Calculate therefore the **CORRELATION TIME** by considering the **autocorrelation functions**:

$$C_M(t) = \langle M(t)M(0) \rangle - \langle M \rangle^2, \quad C_E(t) = \langle E(t)E(0) \rangle - \langle E \rangle^2$$

$$(C_M(0) \propto \chi, \quad C_E(0) \propto C_V)$$

$C_M(t) \rightarrow 0$  and  $C_E(t) \rightarrow 0$  exponentially for  $t \rightarrow \infty$

with a certain decay time  $\tau$ : consider intervals longer than  $\tau$  for statistical averages

(NOTE: "critical slowing down" for  $T \rightarrow T_C$ )

# Measuring physical quantities: how to accumulate data?

## Further remarks...

- see also CORRELATION LENGTH between magnetic domains,  $\zeta(T)$
- close to  $T_c$ , also the correlation length increases (spin alignments are more correlated), up to divergence

# Measuring physical quantities: which errors?

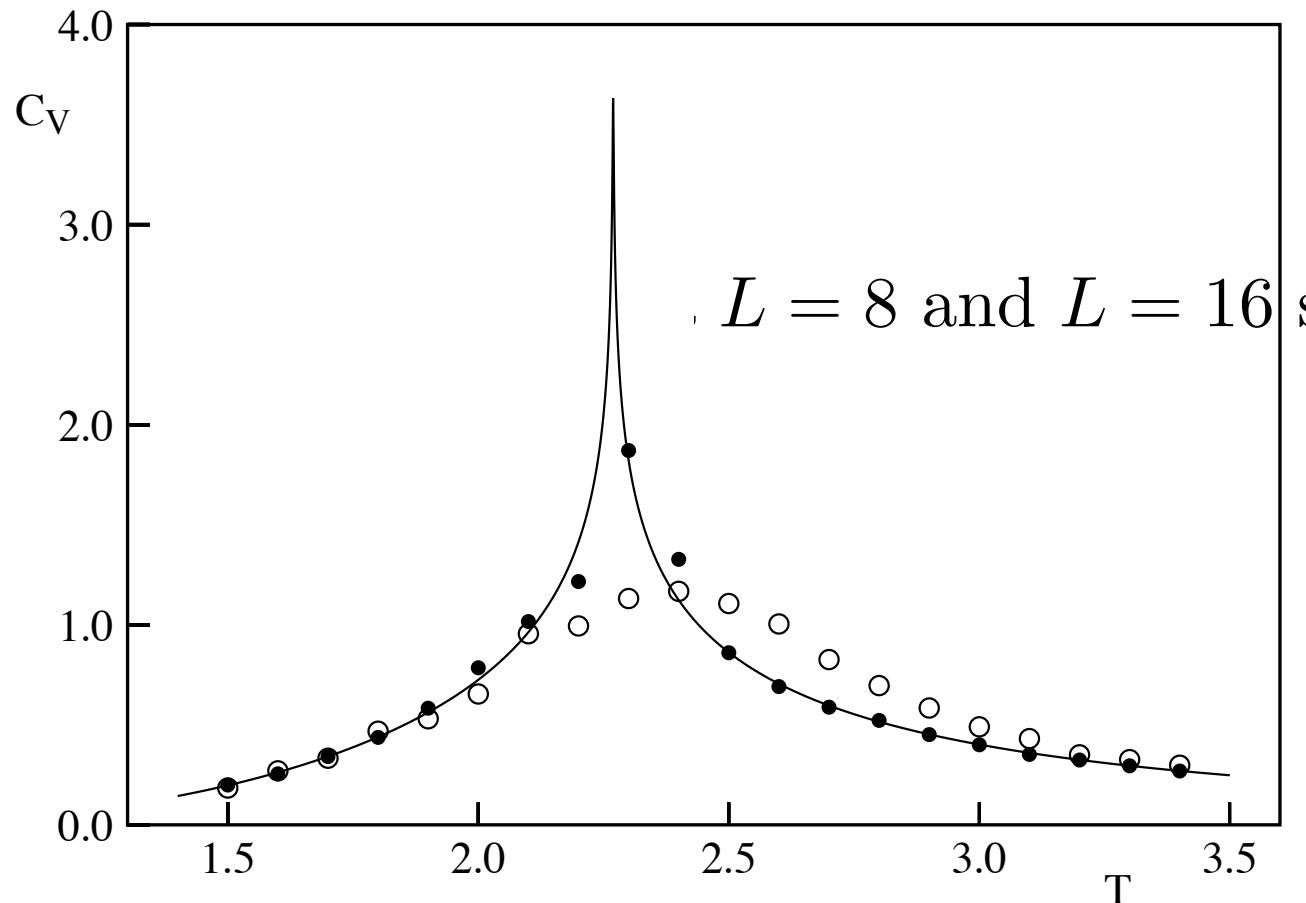
- necessary to give the ERROR ESTIMATE corresponding to the measured physical quantity (see Tab. I of PRB by Landau) !!!
- do also BLOCKING (called “coarse grained technique” in that paper)

# How to do efficiently simulations as a function of T?

- Sometimes EQUILIBRATION time is long...
- IDEA: for  $T'$  close to  $T$ , choose as starting point the equilibrated output of  $T$

# Ising model: size problems

We cannot simulate an INFINITE system!



The temperature dependence of the specific heat  $C$  (per spin) of the Ising model

# Ising model: size problems

SURFACE EFFECTS:

example of energy for HALF UP/HALF DOWN configurations:

$$L=2 \quad E= 0$$

$$L=4 \quad E=-1$$

$$L=8 \quad E=-1.5$$

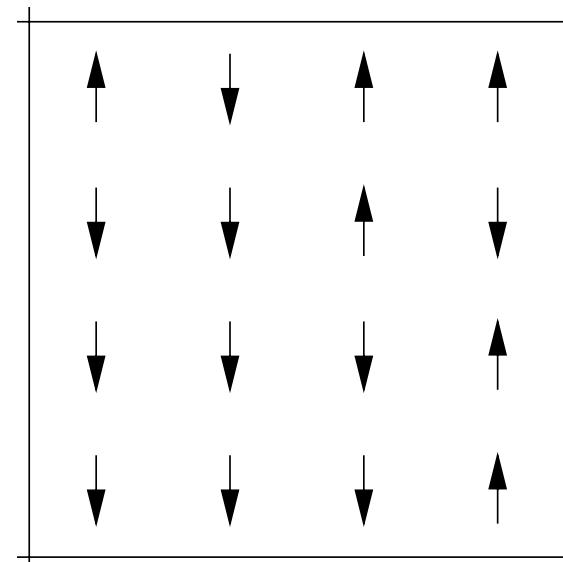
$$L=16 \quad E=-1.75$$

$$L=20 \quad E=-1.8$$

$$L=32 \quad E=-1.875$$

.... for an infinite system:  $E=-2$

We have a (“surface”) term proportional to  $1/L$



# Ising model: alternative dynamics

- in the **SPIN FLIP dynamics** the order parameter is not conserved (**M changes** during evolution)
- alternative: **NN spin exchange (Kawasaki dyn.)** (exchange two NN spins picked at random; **M is conserved**; this is equivalent to LATTICE GAS MODELS with fixed number of particles)

# Ising model: Kawasaki dynamics

Fixed magnetization : change of thermodynamical ensemble

No modification of the equilibrium properties

except phase separation



# Ising model: other generalizations

- SPINS: XY, Heisenberg, Potts...
- LATTICES: Square, Triangle, Cubic, Honeycomb, Kagome....
- INTERACTIONS: Magn. Field, Antiferrom., Next Nearest Neighbor (NNN)....

# Universality and critical exponents

Reduced temperature :  $\Delta T = (T - T_c)/T_c$

$$C \sim |\Delta T|^{-\alpha}$$

$$\langle M \rangle \sim |\Delta T|^{\beta} \quad \text{for } \Delta T < 0$$

$$\chi \sim |\Delta T|^{-\gamma}$$

$$\xi \sim |\Delta T|^{-\nu}$$

# Program:

on

**\$/home/peressi/comp-phys/IX-isng/**

[do: \$cp /home/peressi/.../IX-isng/\* .]

or (for this week) also on:

**\$/home/peressi/public\_html/**

accessible also with a browser at the address:

<http://www.infis.units.it/~peressi/>

**ising.f90**