Ising Lattice

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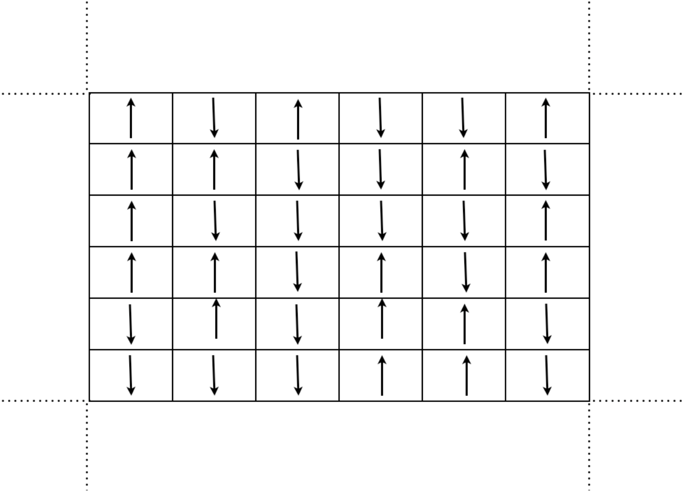
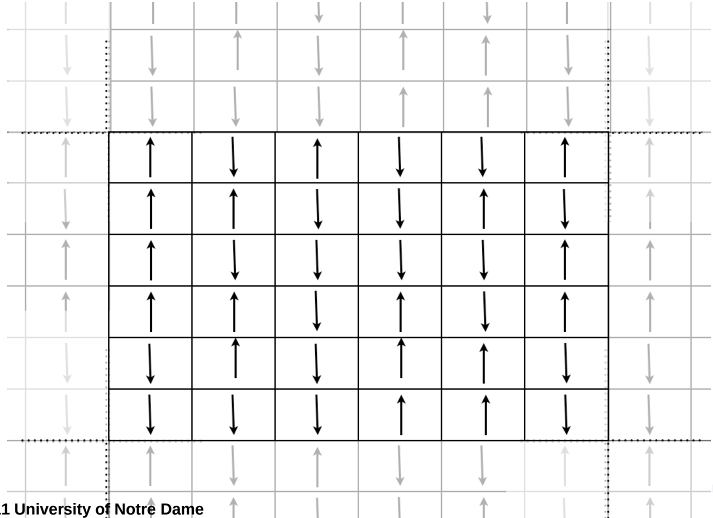
Ising Lattice Model

- Consider a 2-D lattice of "spins" up or down



Ising Lattice Model

- We replicate in all directions to add “periodic boundary conditions”



Ising Lattice Model

Consider a system of N spins on a lattice. In the presence of an external magnetic field, H, the energy of a particular state ν is

$$E_\nu = -\sum_{i=1}^{N} H s_i - J \sum_{ij} s_i s_j \tag{1}$$

- First term: energy due to individual spins coupling with external field
- Second term: energy due to interactions *between* spins.
- Assume that only nearest neighbors interact
- J is *coupling constant*, and describes the interaction energy between pairs.
- When $J > 0$, it is energetically favorable for neighboring pairs to be aligned.

Ising Lattice Model

If J is large enough (or temperature low enough), the tendency for neighboring spins to align will cause a cooperative phenomena called *spontaneous magnetization*.

- Physically: caused by interactions among nearest neighbors propagating throughout the system
- A given magnetic moment influences alignment of spins separated by a large distance
- Such long range correlations associated with long range order; lattice can have net magnetization *in the absence of external magnetic field*.
- Magnetization defined as

$$< M >= \sum_{i=1}^{N} s_i \qquad (2)$$

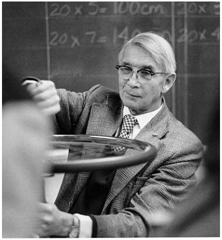
- A non–zero $< M >$ when $H = 0$ is called *spontaneous magnetization*

Ising Lattice Model

- Temperature where system exhibits spontaneous magnetization is the *Curie temperature* (or critical temperature), T_c
- T_c is the highest temperature for which there can be a non–zero magnetization in the absence of an external magnetic field
- For $T_c > 0$, Ising model undergoes an *order–disorder transition*
- Similar to a phase transition in a fluid system - simple model of a fluid
- No order-disorder transition in 1-D only 2-D and 3-D

Ising Lattice Model

- 1-D Ising model solved analytically by Ernst Ising in his 1924 PhD thesis



  - Historical note: German Jew who fled Europe, ending up in Peoria, IL as physics teacher at Bradley University
  - Never published again after WWII
  - Died in 1998 - see obituary: http://www.bradley.edu/las/phy/personnel/isingobit.html

Ising Lattice Model

Lars Onsager showed in the 1940s that for $H = 0$, the partition function for a two–dimensional Ising Lattice is

$$Q(N, \beta, 0) = [2\cosh(\beta J) e^{I}]^{N} \tag{3}$$

where

$$I = (2\pi)^{-1} \int_0^{\pi} d\phi \ln(\frac{1}{2}[1 + (1 - \kappa^2 \sin^2 \phi)^{1/2}])$$

with

$$\kappa = 2\sinh(2\beta J)/cosh^2(2\beta J)$$

This result was one of the major achievements of modern statistical mechanics

Ising Lattice Model

- It can be shown that

$$T_c = 2.269J/k_B \tag{4}$$

- Furthermore, for $T < T_c$, the magnetization scales as

$$\frac{M}{N} \sim \alpha(T_c - T)^{\lambda} \tag{5}$$

- Should be possible to perform Metropolis simulation of this!

Properties of Ising Lattice

- Physically, Ising lattice shows many of the characteristics of a fluid
- Magnetic susceptibility, $\chi = (< M^2 > - < M >^2)/k_B T$, diverges at critical point
- Local magnetization fluctuations become very large near critical point, similar to density fluctuations near critical point of a fluid
- Small variations in $k_B T/J$ lead to spontaneous phase changes

Properties of Ising Lattice

- The *correlation length* (distance over which local fluctuations are correlated) is unbounded at T_c

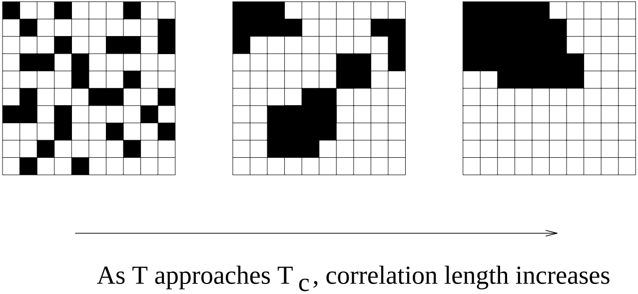


Figure: T_c is being approached from left to right. The correlation length of like regions (i.e. black and white squares) increases. At T_c, an order–disorder transition occurs, analogous to condensation

Ising Lattice Algorithm

How to simulate the 2-D Ising lattice?

1. Choose an initial state of spins (it will not matter)
2. Choose a site i
3. Calculate the change in energy ΔE if the state if i is changed
4. If energy is lowered by change, accept the change. If not...
5. Generate random number $0 < \zeta < 1$
6. If $\zeta < \exp(-\beta \Delta E)$ accept the change. Otherwise, don't
7. Repeat

Compute $< M >$, $< E >$ and fluctuations versus T. Let's do it!

Ising interactive Algorithm

Take a look at the source code ising2d.f

- Lattice array or 0 or 1:

  `latt(ix,iy)`
- Largest allowable lattice size: 40 X 40
- Initialize it in one of four choices
- Compute the initial energy

  `CALL echeck`

Ising interactive Algorithm

Core Metropolis algorithm is in routine “update”

```
 do istep=1,nstep
    CALL update

ccc  sum E, M and fluctuations
      emean=emean+etot
      efluc=efluc+etot*etot
      rmmean=rmmean+dfloat(mtot)
      rmfluc=rmfluc+dfloat(mtot)*dfloat(mtot)
 enddo                        ! istep = 1,nstep
```

Ising interactive Algorithm

Metropolis implementation for an nsize X nsize lattice

```
   size=dfloat(nsize)
   nsize1=nsize-1

ccc Pick a spin at random. Each call to
ccc update performs nsize^2 attempts

   do iflip=1,nsize*nsize
ccc  (ix,iy) is a random position on lattice
     ix=int(size*uni())+1
     iy=int(size*uni())+1

ccc nhsum is a counter that sums the value
ccc of all spins adjacent to (ix,iy)
     nhsum=0
```

```
ccc   get positions adjacent to (ix,iy)
ccc  (remember PBC)
      do nhbr=1,4
        nhx=mod(ix+nhxl(nhbr)+nsize1,nsize)+1
        nhy=mod(iy+nhyl(nhbr)+nsize1,nsize)+1
        nhsum=nhsum+latt(nhx,nhy)
      enddo

ccc    compute energy felt by spin at (ix,iy)
       itest=nhsum*latt(ix,iy)
```

Here is the Metropolis algorithm

```
if (itest.le.0) then
ccc Automatically accept the move
ccc Sum total energy and magnetization
     mtot=mtot-2*latt(ix,iy)
     latt(ix,iy)=-latt(ix,iy)
else
ccc  Select a random number on (0,1)
ccc  Conditional accept (embe is precalculated E)
    if (test.le.embe(itest)) then
      etot=etot+dfloat(itest)*rj2
      mtot=mtot-2*latt(ix,iy)
      latt(ix,iy)=-latt(ix,iy)
    end if
ccc     Reject the move. Keep everything the same
  end if
```

Ising interactive

- Run Ising interactive at $T > T_c$. Note the value of the magnetization , fluctuations
- Dump the configuration and look at it. What do you see?
- Slowly reduce T and approach T_c. What happens?
- Start at low T ($T \approx 0.4$). What happens?
- Slowly raise T to approach $T_c = 2.26$ What happens?

Ising batch input file

```
ising.40.10K.log : name of log file
123456           : rdm nbr seed
mvst.1           : magnetization vs T filename
75               : unit (don't change)
evst.1           : energyvs T filename
76               : unit (don't change)
mflucvst.1       : magnetiz fluc vs T filename
77               : unit (don't change)
eflucvst.1       : energy fluc vs T filename
78               : unit (don't change)
1                : 1=random,2-inter,3=check,4=read
5000             : number of equilibration steps
2                : n different runs
40 10000 4       : nsize nstep kT/J for run
40 10000 2       : nsize nstep kT/J
```