ISING MODEL & SIMULATION

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(Fall 2008)

Ising Model & Simulation (Fall 2008)

This presentation demonstrates the main idea of Ising Model as a standard model in statistical mechanics.

I have to view the structure of my simulation and introduce the Metropolis Algorithm which is necessary in Ising Models simulations.

Finally, as a conclusion, I compare the analytical solutions and the computational simulation result.

- Ising Model
- Simulation
- Metropolis Algorithm
- Conclusion

ISING MODEL

What is the problem?

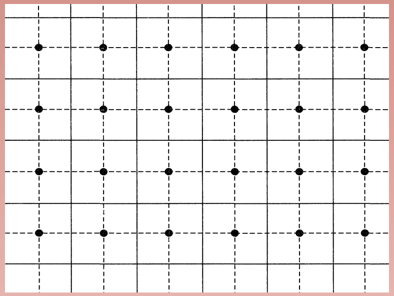
- ✓ The theoretical description of phase transitions
- ✓ The phase transition of ferromagnets at the Curie temperature

  Ferromagnetic materials, when heated, eventually lose their magnetic properties. This loss becomes complete above the *Curie temperature*, named after the French physicist Pierre Curie, who discovered it in 1895. (The Curie temperature of metallic iron is about 770° C.)
- ✓ The order-disorder transition in a binary alloy
- ✓ The spin glass in many-particle Physics (Crystalline-Amorphous transition of metals)
- ✓ The human brain problem and schematic neural networks

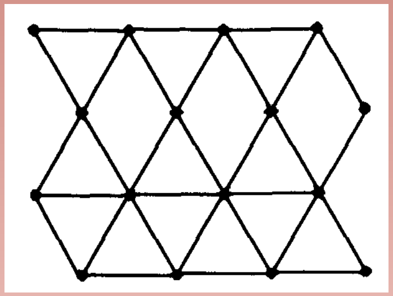
What is the main ideas of Ising model?

- ✓ Heisenberg Model: XYZ
- ✓ Ising model:
  - ✓ Only one direction orientations $\sigma_z=\pm1$
  - ✓ First neighbor interaction
  - ✓ $H=-\sum J(\sigma_i \sigma_j-1)$
  - ✓ Periodic Lattice
- ✓ 1-D & 2-D has exact solution

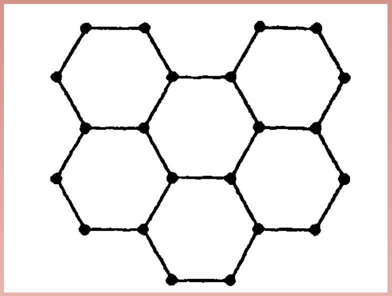
Three Stucture in 2-D



Square (4)



Traingular (6)



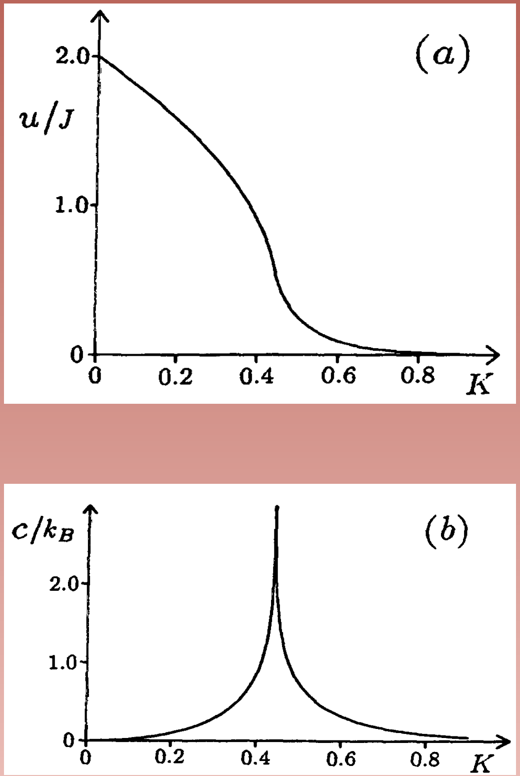
Hexagunal (3)

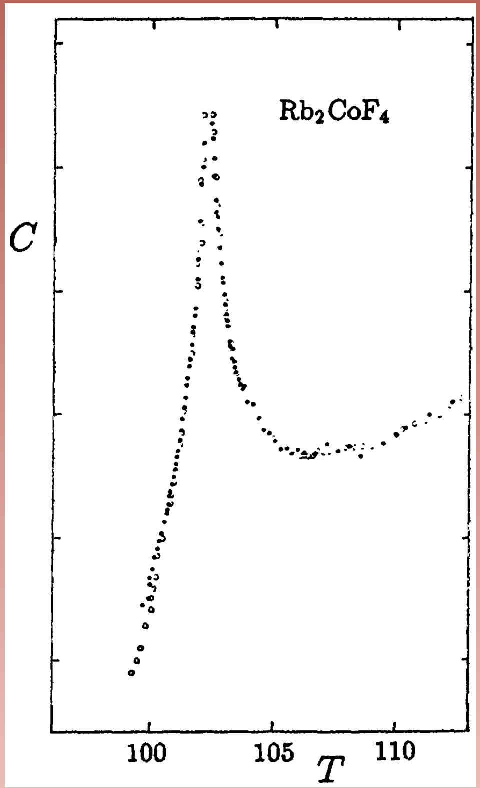
- ✓ This simulation is 2-D Ising Model with Square lattice

Exact Solution

- ✓ Reichl, L.E., “A Modem Course in Statistical Physics”, 2nd edition, John Wiley & Sons, (1998), 462-485.

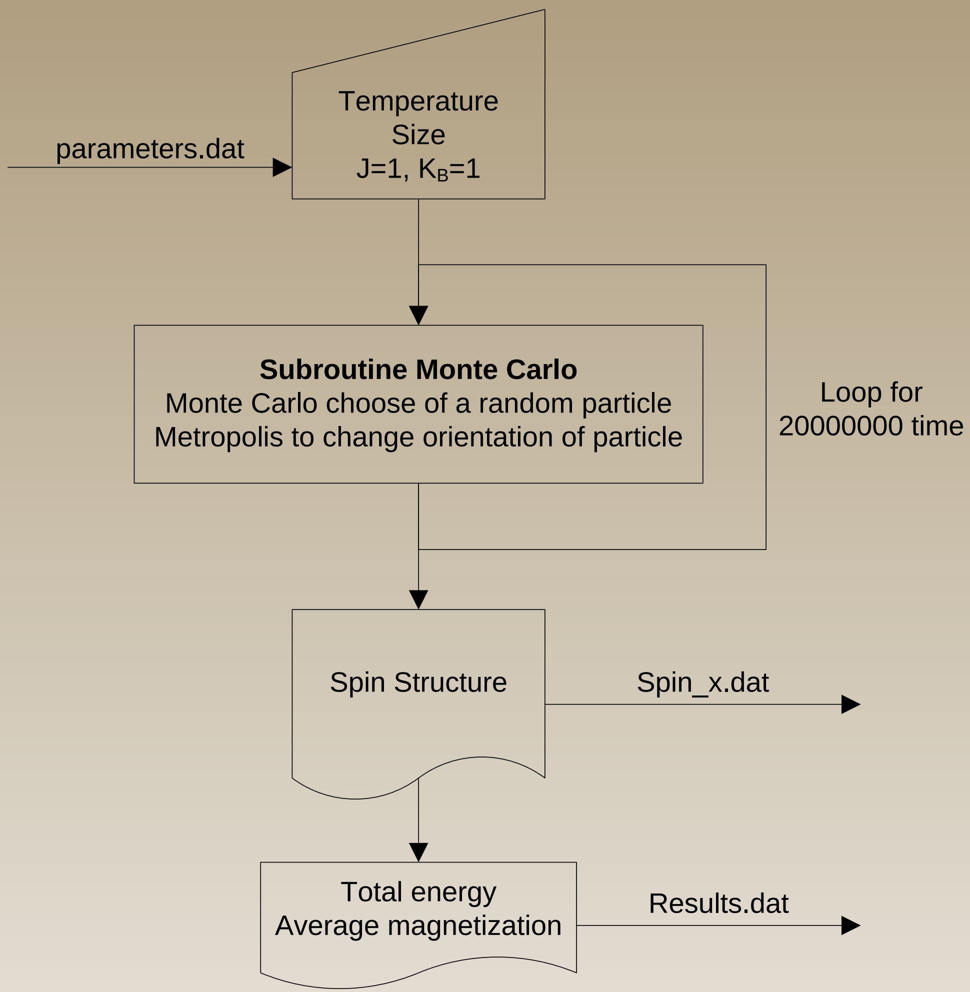
- ✓ T_C=2.269 j/k_B
- ✓ K_C=0.4407 k_B/j





SIMULATION

Simulation Algorithm



METROPOLIS ALGORITHM

Metropolis Algorithm

- ✓ Statistical Condition of Transitions : Boltzmann Factor

$$P(A \to B) \propto \frac{e^{\left(-\frac{\varepsilon_B}{k_B T}\right)}}{e^{\left(-\frac{\varepsilon_A}{k_B T}\right)}} = e^{\left(-\frac{\Delta\varepsilon}{k_B T}\right)}$$

- ✓ Annealing Algorithm:
  - ✓ Target: The change of equilibrium with temperature
  - ✓ Heating and cooling it slowly
  - ✓ Step 1: Initial Condition
    - ✓ Disordered: hot start
    - ✓ Ordered: cold start
  - ✓ Step 2: Repeatly apply the algorithm of thermal equilibrium
- ✓ Landau, R. and Paez , M. J. "Computation Physics : Problem Solving with Computers", John Wiley & Sons, (1976), 297-305.

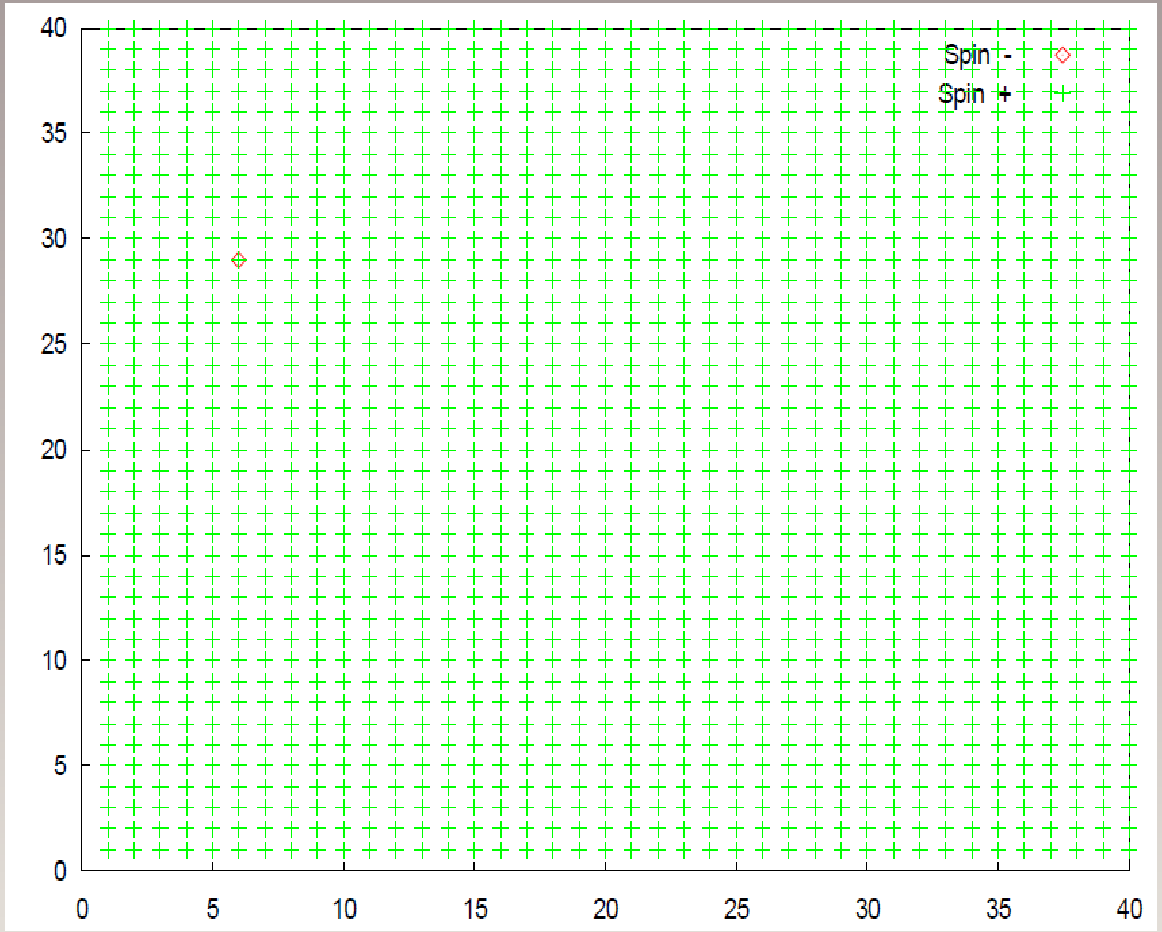
Metropolis Algorithm

1. Start with an arbitrary spin configuration: $\{s_{ij}\}$
2. Generate a new state
   1. Choose ij^{th} element randomly
   2. Reverse ij^{th} spin direction to create a trial configuration
   3. Calculate the energy of the trial configuration
   4. If $E_{new} < E_{\{sij\}}$ then accept the change
   5. Else with random process with P probability accept the change

CONCLUSION

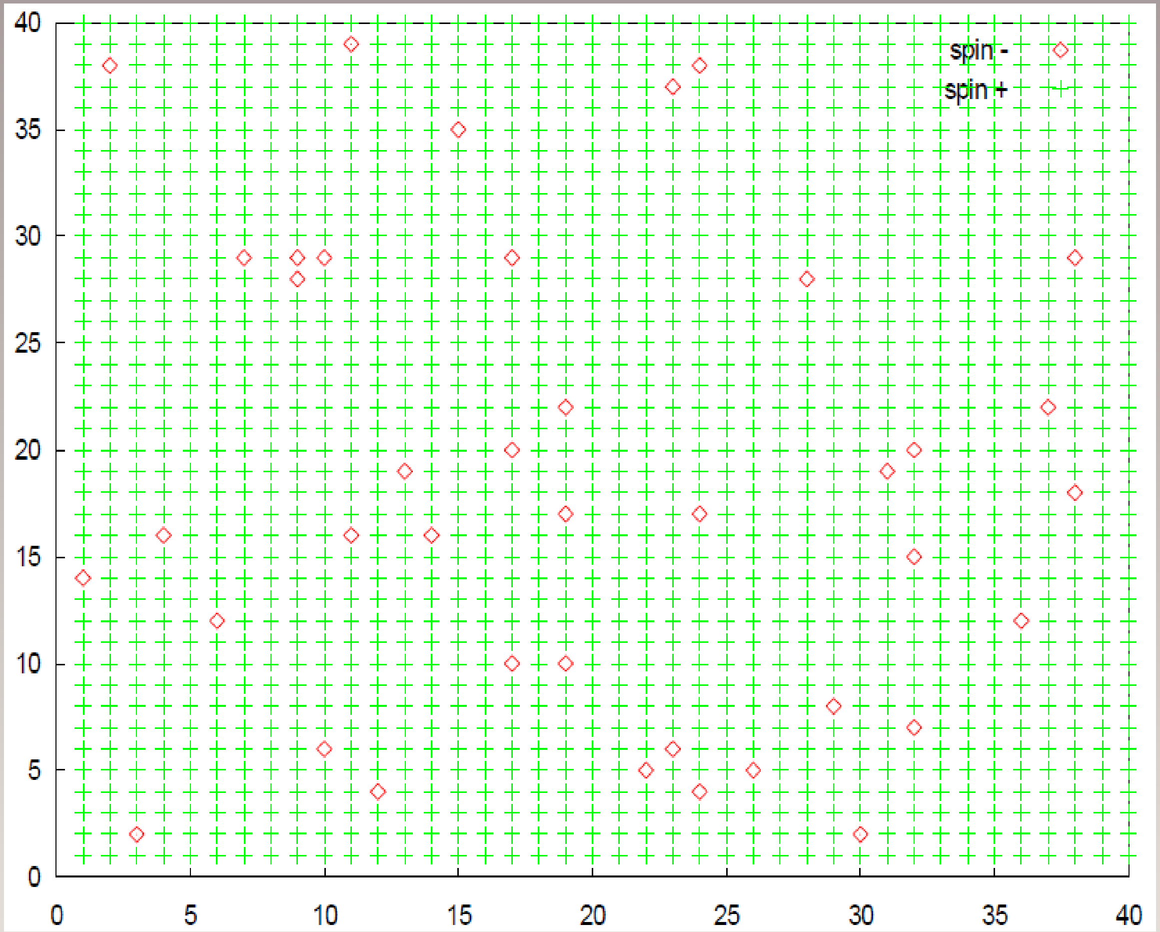
Structure in 40×40 Lattice T=0.1

Average Magnetization = 1



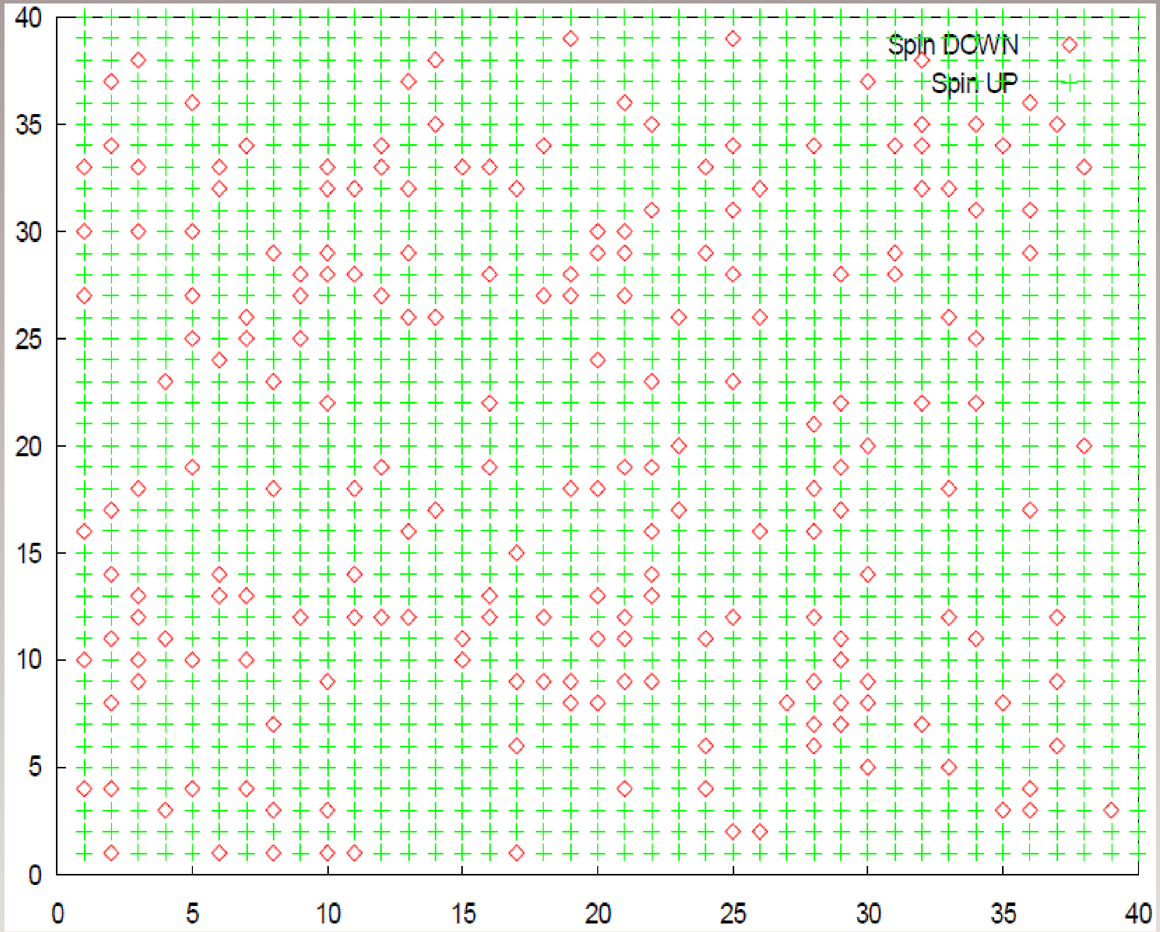
Structure in 40×40 Lattice T=1.0

Average Magnetization = 0.9446



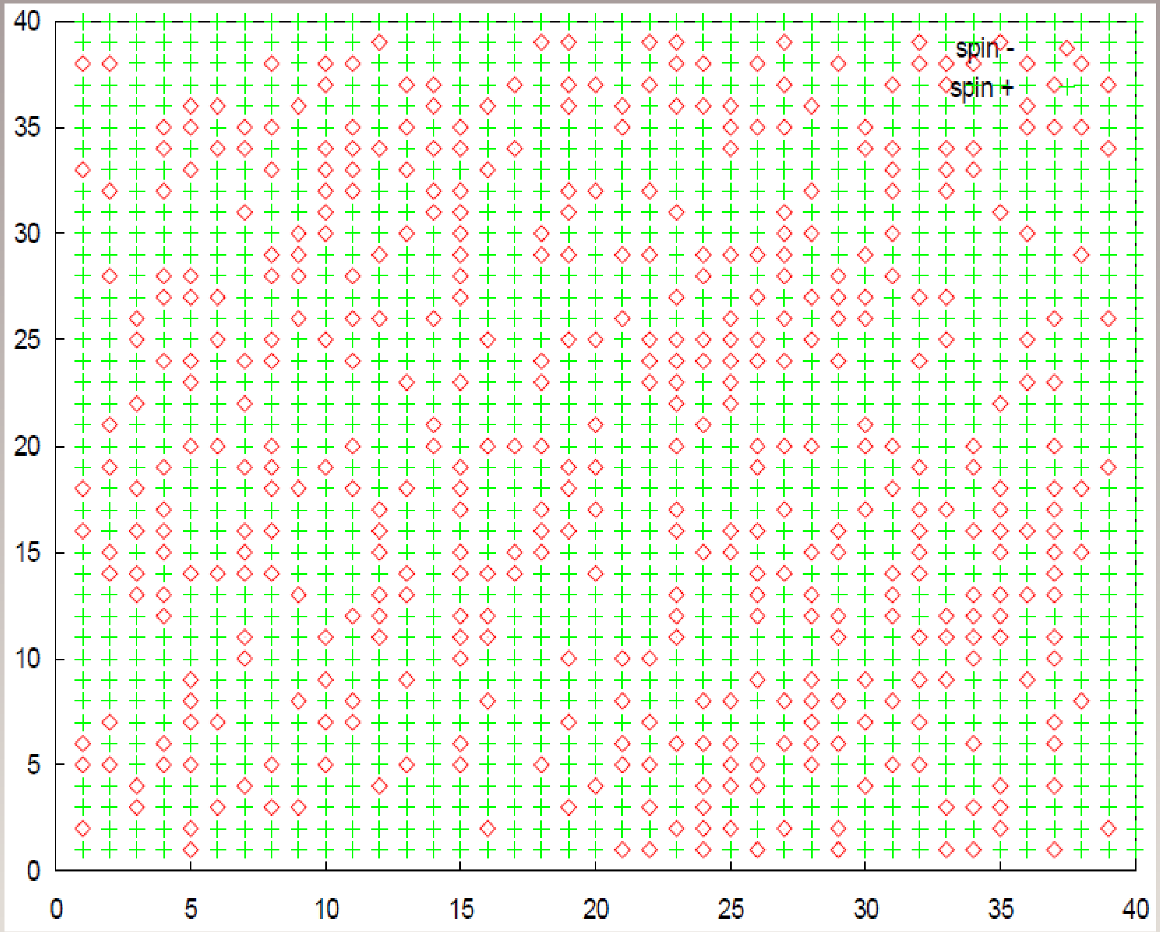
Structure in 40×40 Lattice T=1.5

Average Magnetization = 0.7316



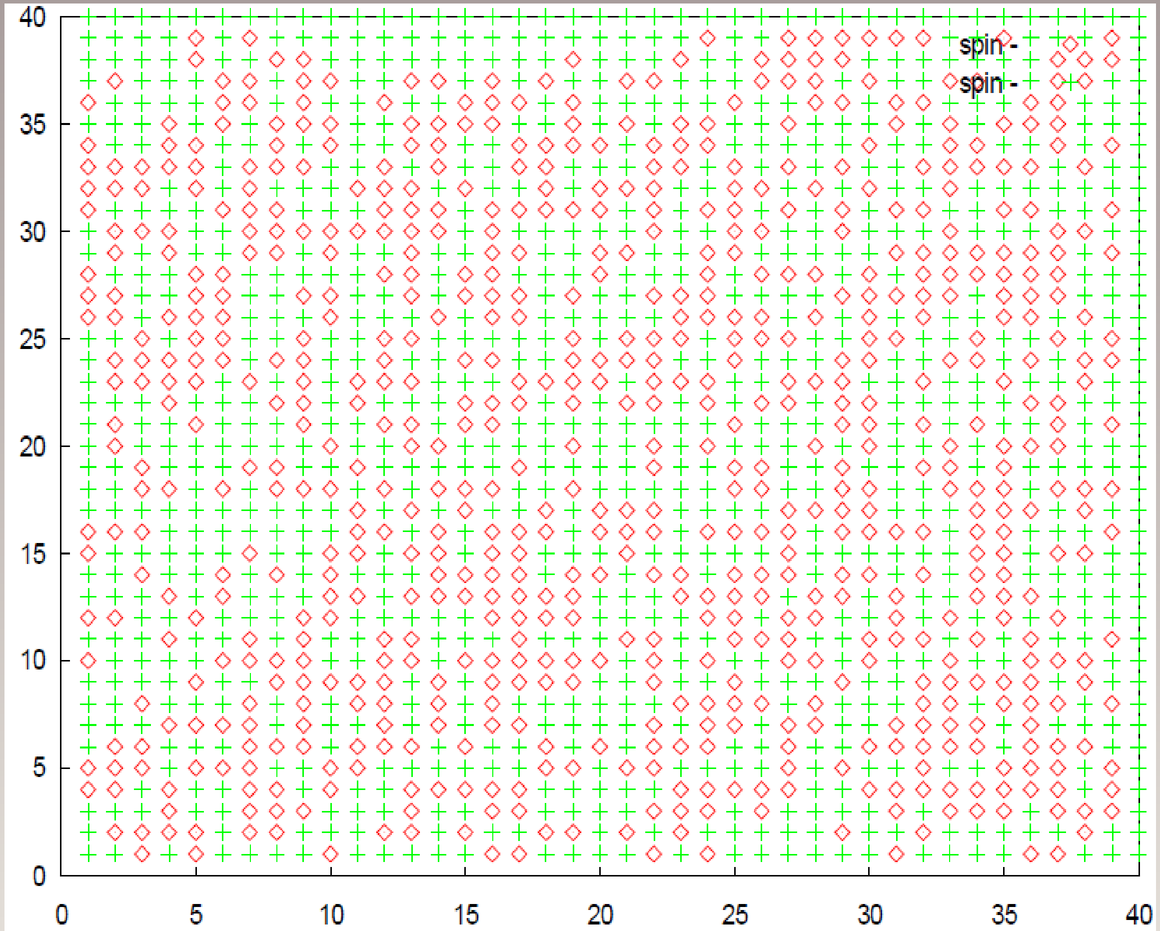
Structure in 40×40 Lattice T=2

Average Magnetization = 0.3589

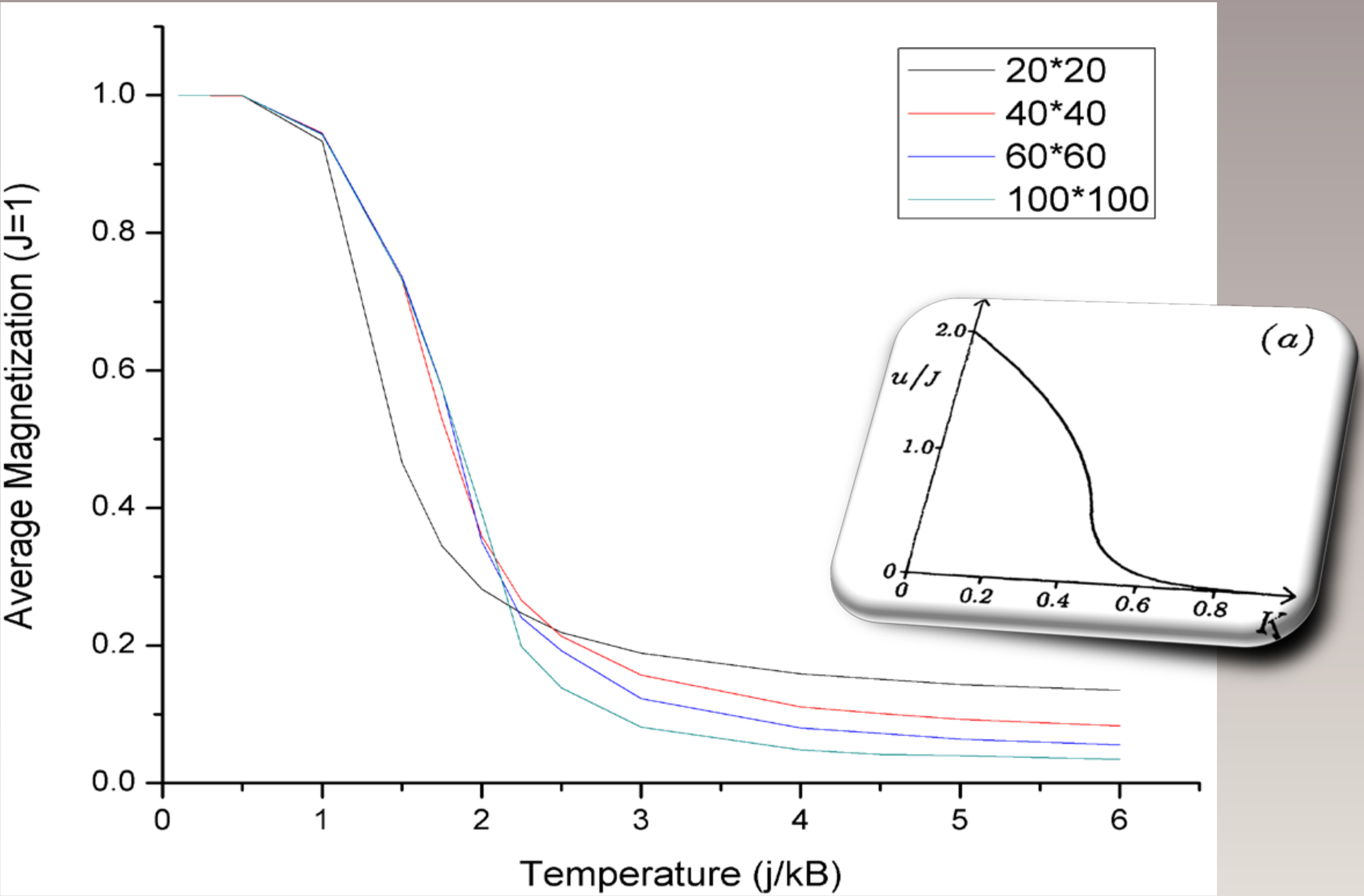


Structure in 40×40 Lattice T=4

Average Magnetization = 0.1107



Simulation Results $T_C \approx 2.1\ j/k_B$



BEST WISHES!