Monte Carlo Simulations in Statistical Physics: Phase Transitions in the Ising Model of Magnetism

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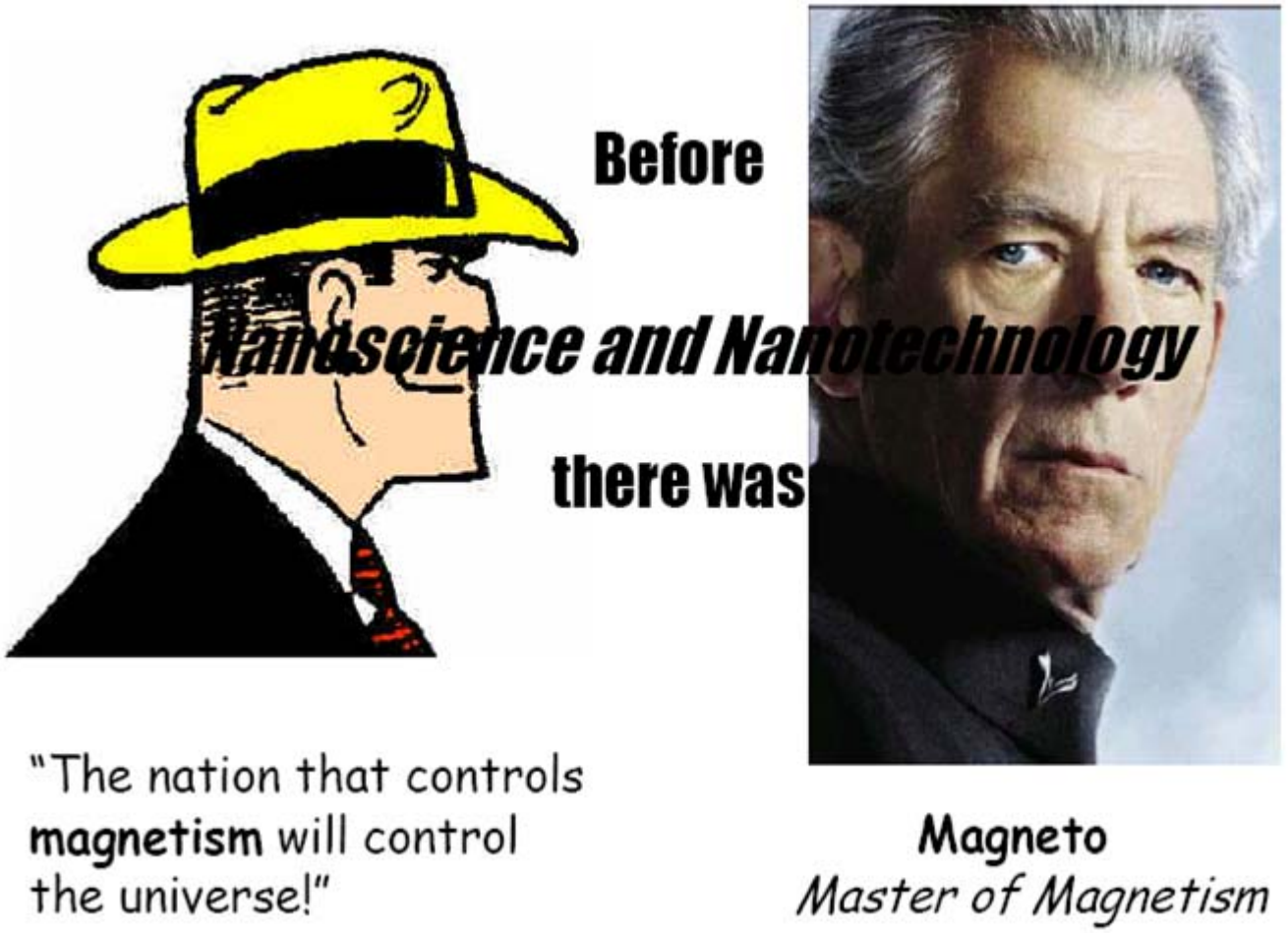
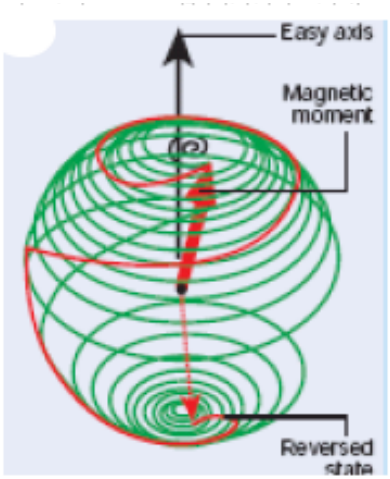
PHYS 460/660: Computational Methods of Physics

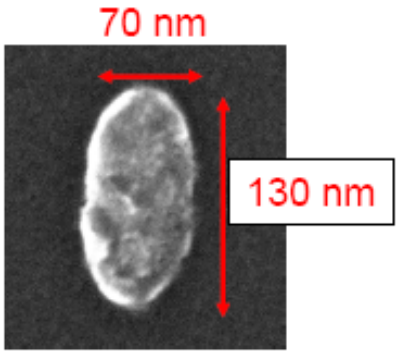
http://wiki.physics.udel.edu/phys660

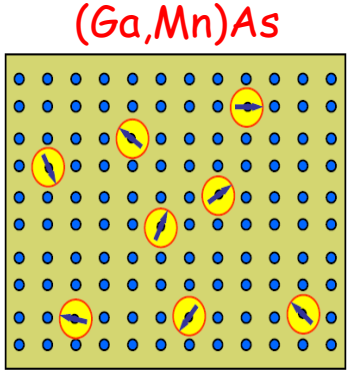
Magnetism is One of the Oldest Complex Phenomena Known to Humankind



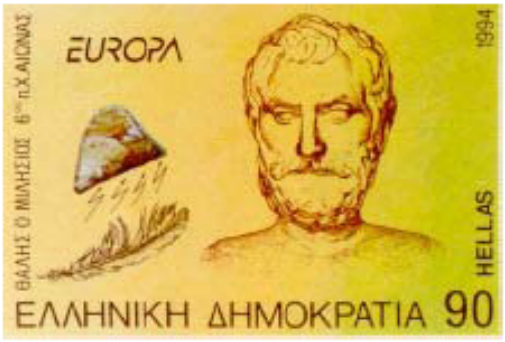
From Lodestones to Nanomagnetism and Semiconductor Spintronics







Lodestone (Chinese – Loving Stone)



Thales of Miletus is credited with discovering that amber rubbed with wool or fur attracts light bodies such as pieces of dry leaves or bits of straw, and **observing that lodestone attracts iron and other lodestones**.

www.phy6.org/earthmag/lodeston.htm

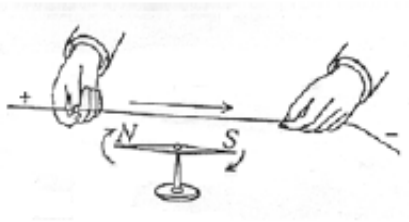
Magnetite A black, isometric, strongly magnetic, opaque mineral of the spinel group, (Fe_3O_4). It constitutes an important ore of iron. Magnetite is a very common and widely distributed accessory mineral in rocks of all kinds

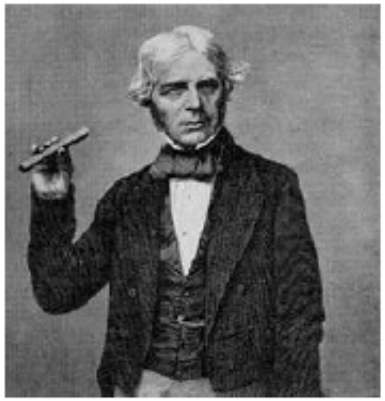
How is magnetite magnetized in nature?

One proposal is that this occurs during lighting strikes when strong fields are generated by the current passing through the mineral.

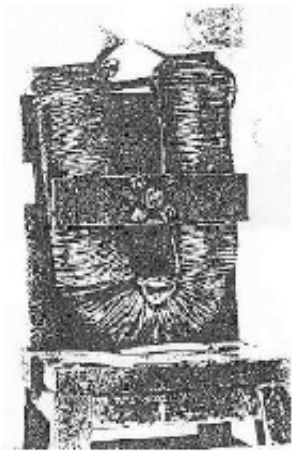
Unification of Electricity and Magnetism

1820 -Oersted discovers that electrical currents create magnetic fields





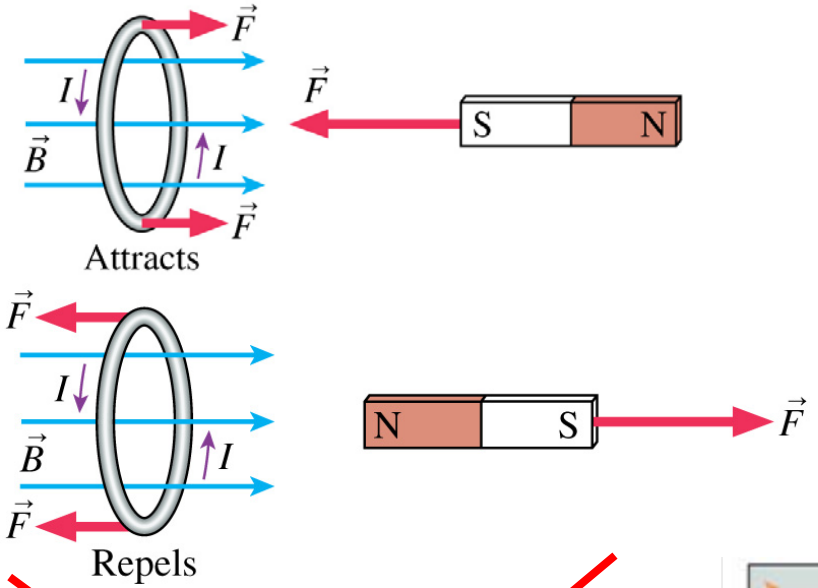
1831 – Faraday discovers that changing magnetic fields create electric fields – Faraday induction

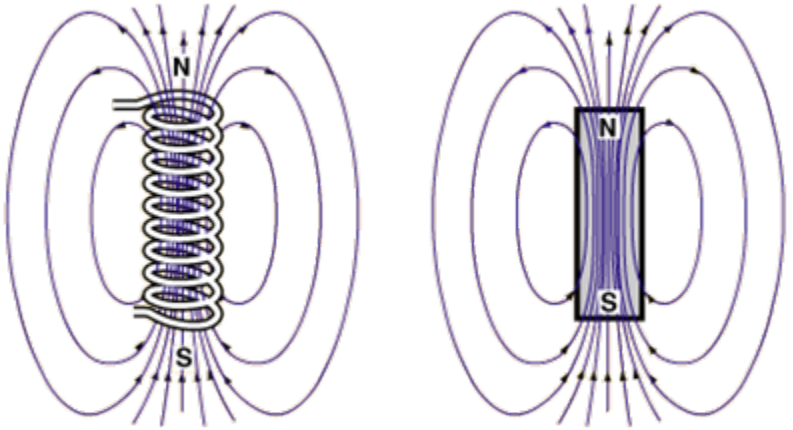


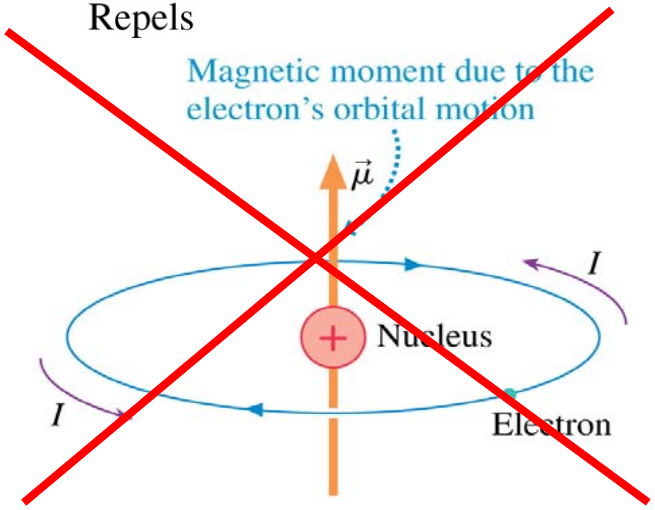
Two results:

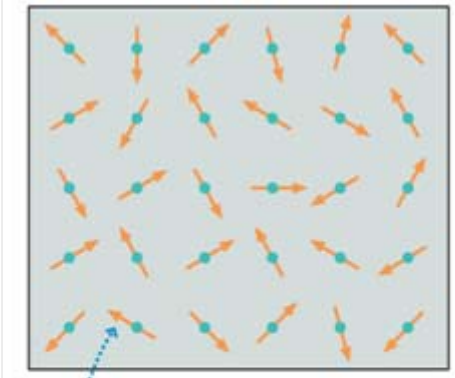
- The development of a fundamental understanding of electromagnetism.
- Strong technological need for better magnetic materials and stronger magnets.

Permanent Magnets vs. Current Carrying Wires: Quantum vs. Classical Physics

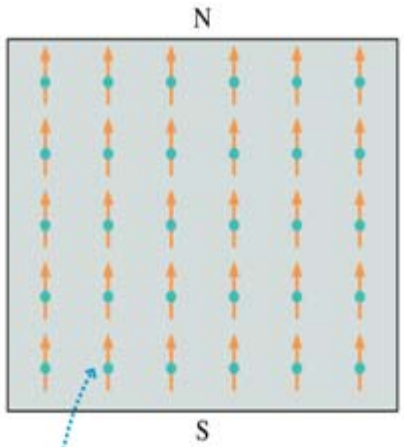








The atomic magnetic moments due to unpaired spins point in random directions. The sample has no net magnetic moment.

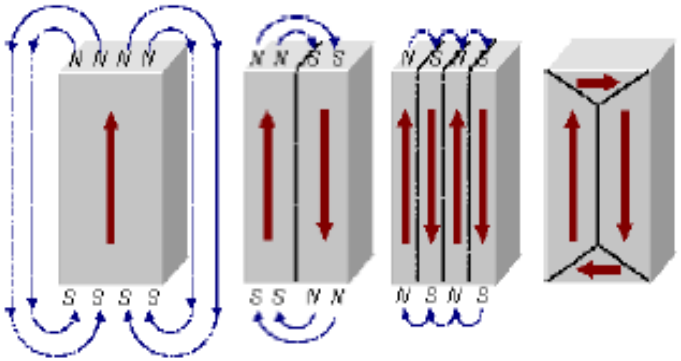


The atomic magnetic moments are aligned. The sample has a north and south magnetic pole.

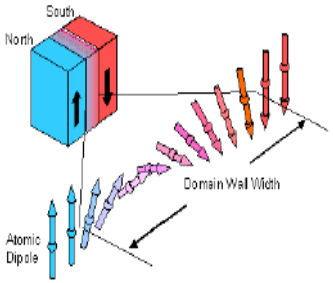
Microscopic Structure of Permanent Magnets

The magnetic energy of a ferromagnet is reduced via the formation of domains

Ideal – single crystal behavior of a magnetically "soft" material →

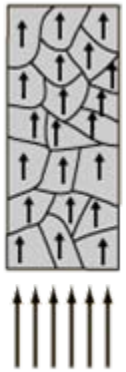


More typically, in polycrystalline ferromagnets domains are irregular in form and not perfectly matched



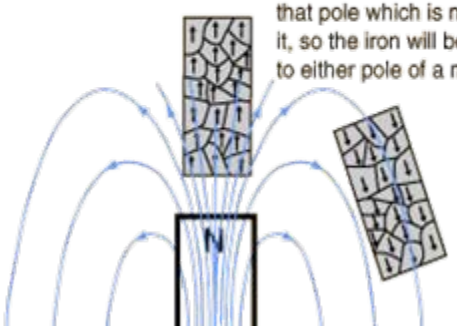
Domain size set by energy cost of forming **domain walls** balanced by the energy reduction by formation of domains
Domain wall thickness ~ 10 – 1000+ nm.

In bulk material the domains usually cancel, leaving the material unmagnetized.

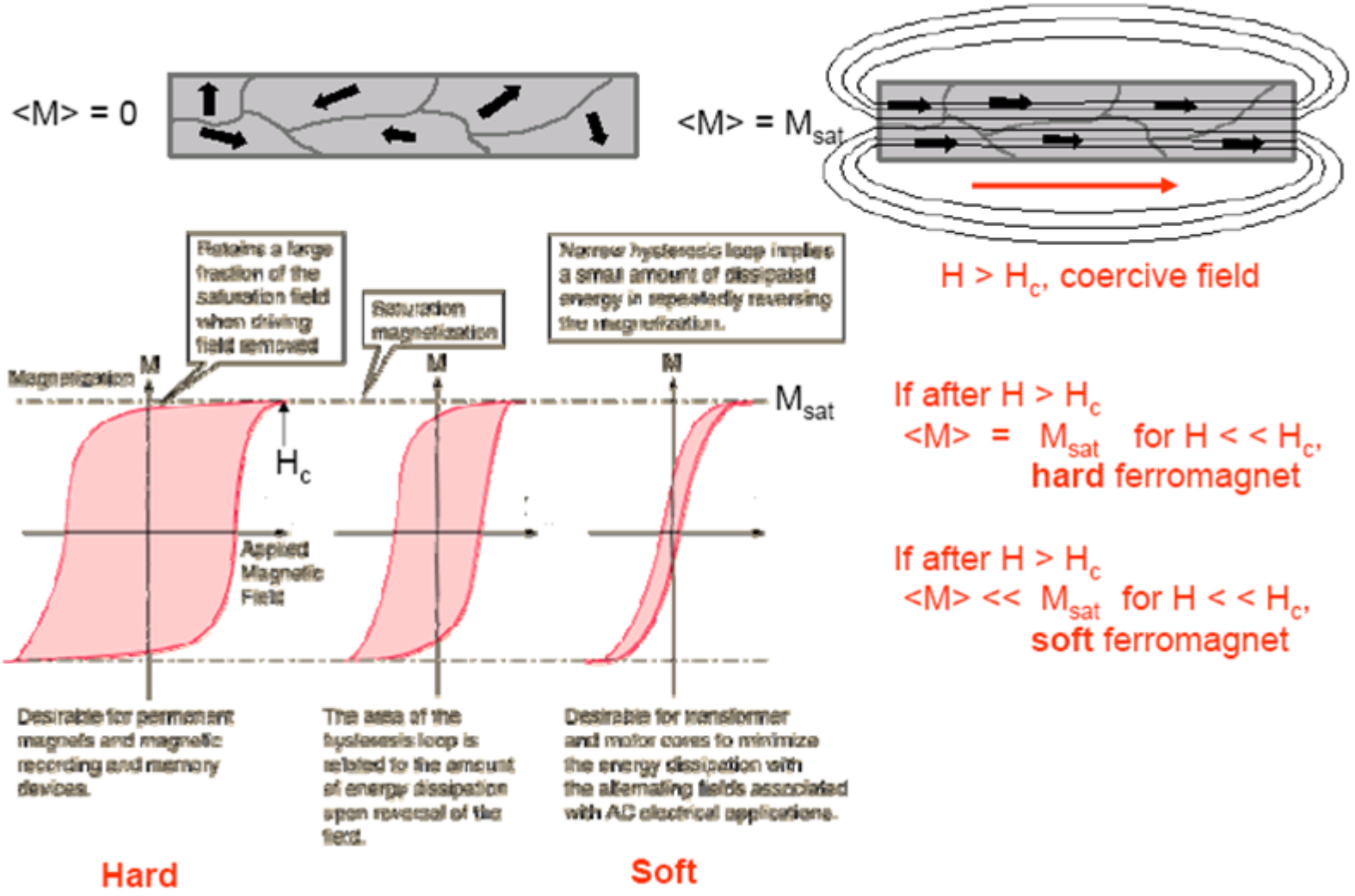


Externally applied magnetic field.

Iron will become magnetized in the direction of any applied magnetic field. This magnetization will produce a magnetic pole in the iron opposite to that pole which is nearest to it, so the iron will be attracted to either pole of a magnet.



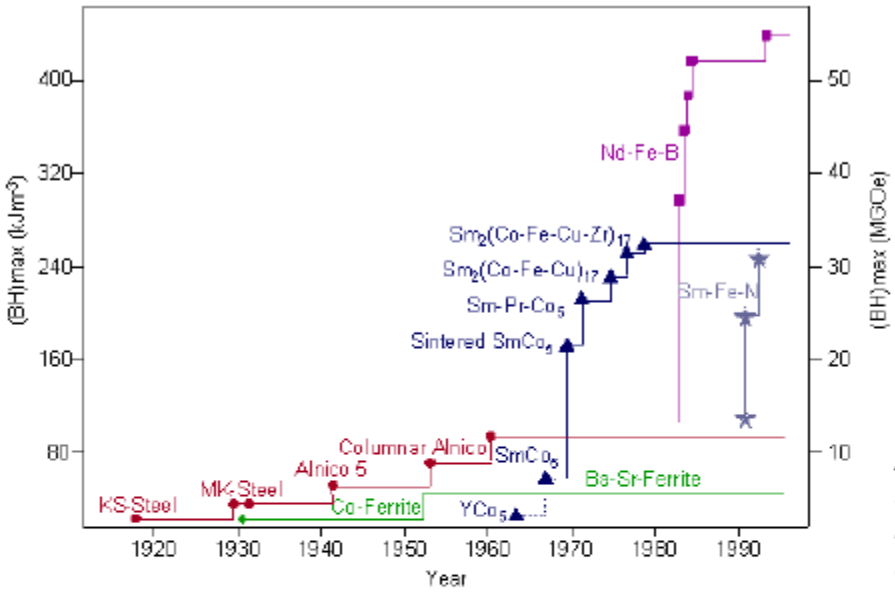
Ferromagnetic Materials: "Hard" vs. "Soft"



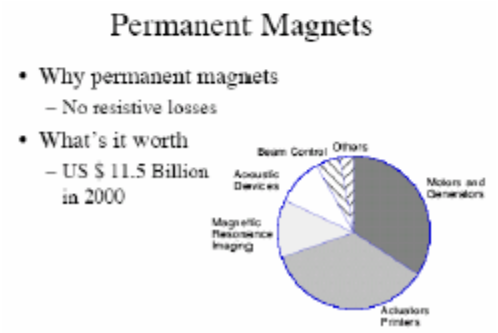
If after $H > H_c$
$\langle M \rangle = M_{sat}$ for $H << H_c$,
hard ferromagnet

If after $H > H_c$
$\langle M \rangle << M_{sat}$ for $H << H_c$,
soft ferromagnet

Development of (Hard) Ferromagnetic Materials



A lodestone magnet from the 1750's and typical ferrite and rare earth used in modern appliances. Each of these contain about 1J of magnetic energy.



The number of magnets in the family car has increased from one in the 1950's to over thirty today.

Over 30g of magnets are produced annually for each person on Earth.

Quantum Mechanics of Magnetism Summarized

- Due to the motion of their electrons, some atoms can have intrinsic magnetic moments. Other atoms develop magnetic moments when placed in an external magnetic field.

- If atoms have zero magnetic moment, then an applied field H induces magnetic moments that are aligned anti-parallel to the applied field. The magnetization M is such that $M/H < 0$. This is called **diamagnetism.**

- If atoms have non-zero magnetic moments that point in random directions then the sum over many atoms gives zero magnetization. An applied field tends to align the magnetic moments so that $M/H > 0$. This is called **paramagnetism.**

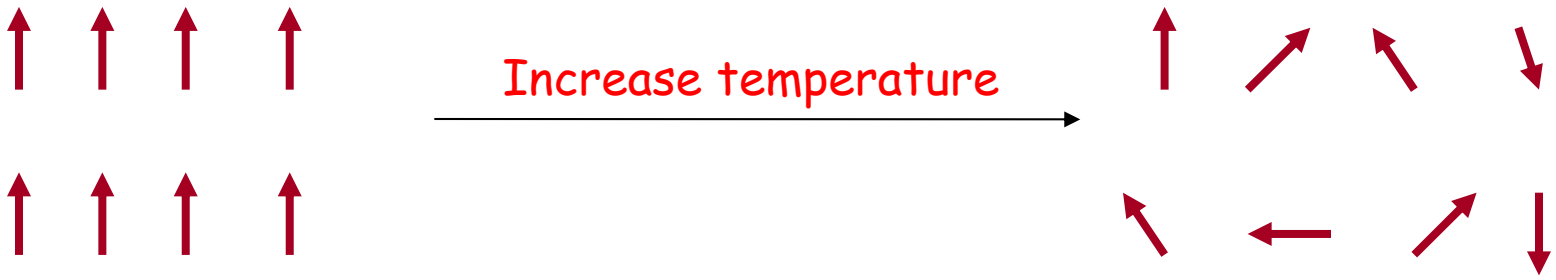
- If atoms have non-zero magnetic moments that point in the same direction then the sum over many atoms gives finite magnetization. This is called **ferromagnetism.**

Bohr-van Leeuwen Theorem: At any finite temperature, and in all finite applied electric or magnetic fields, classical magnetization of a collection of electrons in thermal equilibrium vanishes identically.

Classification of Phase Transitions and Magnetization as the Order Parameter

Ferromagnet:
Spins aligned

Paramagnet:
Spins disordered



- Spontaneous magnetization (in the absence of magnetic field): **Order Parameter**.
- Ordered phase spontaneously breaks spin rotation symmetry.
- **First Order Phase Transitions:** discontinuity in the order parameter or energy (i.e., first derivative of the free energy).
- **Second order Phase Transitions:** divergence in the susceptibility or specific heat (i.e., second derivative of the free energy).

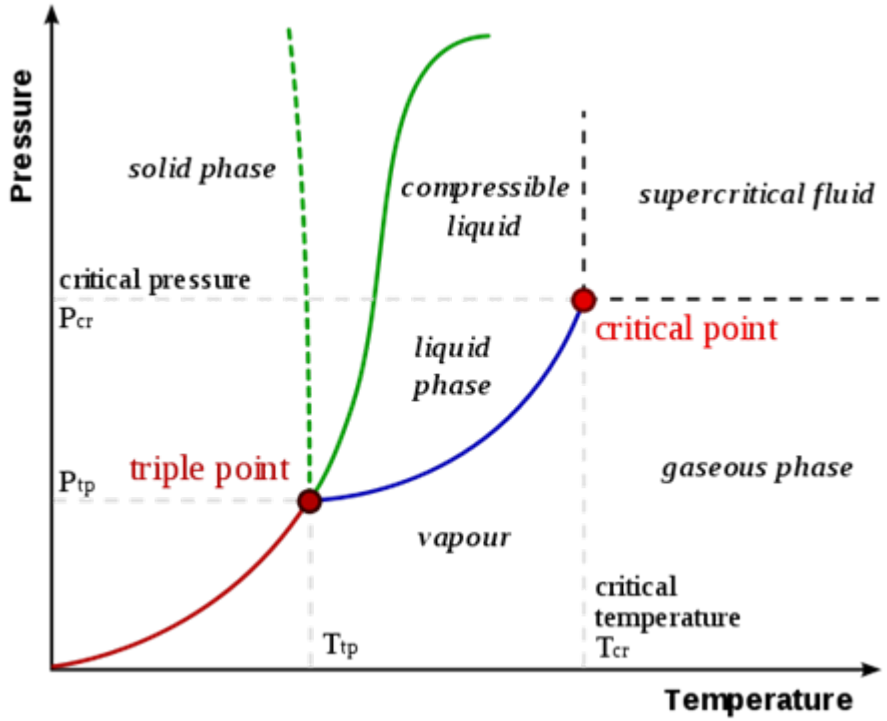
Where Do Phase Transitions Occur?

Energy-Entropy argument:

$$F = E - TS$$

- At high temperature the entropy S always dominates the free energy, and the free energy is minimizes by maximizing S.
- At low temperatures, there is a possibility that internal energy E dominates TS in free energy, and free energy is minimized by minimizing E.
- If the macroscopic state of the system obtained by these two procedures are different, than we conclude that at least one phase transition has occurred at some intermediate temperature.

Familiar Phase Diagram: Liquid-Gas-Solid



The boundary lines between phases are called the coexistence lines. Crossing a coexistence line leads to a **first order** phase transition, which is characterized by a discontinuous change in thermodynamic quantities which are first –order derivative of the free energy, such as **volume, enthalpy, magnetization**.

- Notice that, while the melting curve, in principle, can be extended to infinity, the gas-liquid/boiling curve terminates at a point, beyond which the two phases cannot be distinguished.

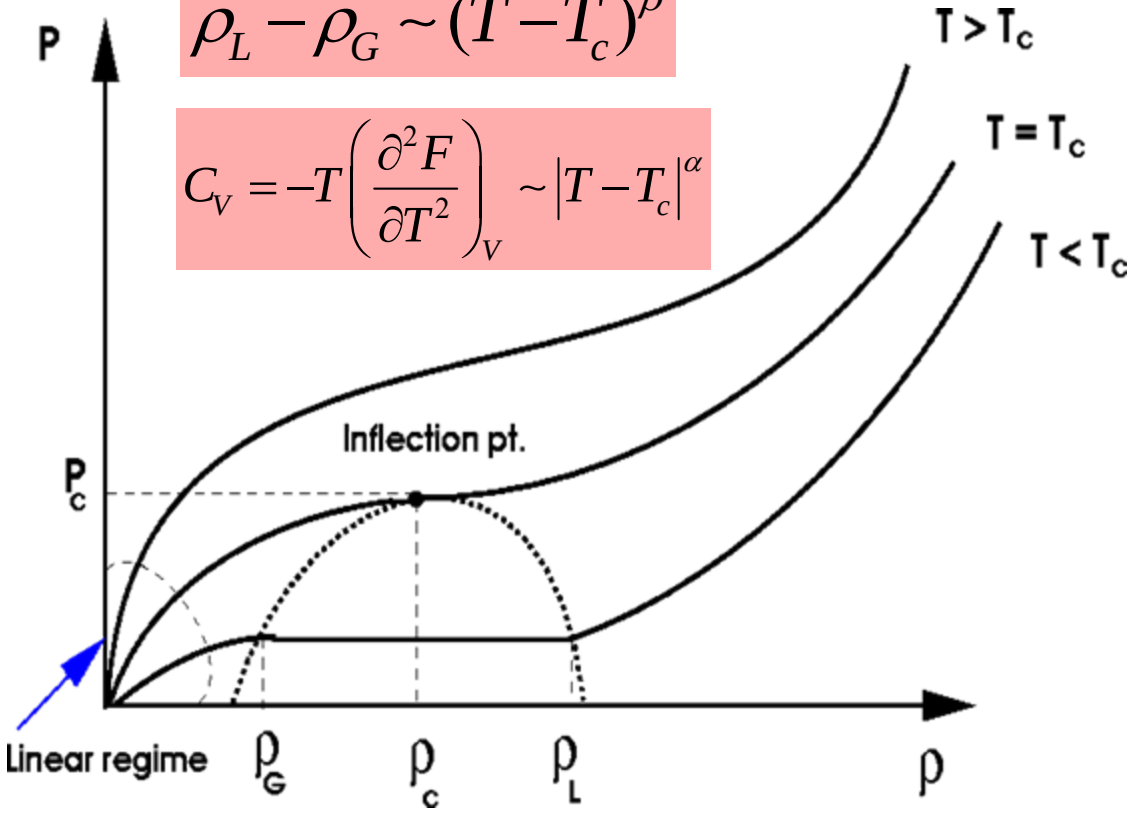
- This point is called a critical point and beyond the critical point, the system is in a supercritical fluid state. The temperature at which this point occurs is called the critical temperature.

- At a critical point, thermodynamic quantities expressed as first-order derivative of the free energy remain continuous, but derivatives of these functions may diverge. Examples of such divergent quantities are the heat capacity, isothermal compressibility, magnetic susceptibility, etc.

Order Parameter and Critical Exponents for Liquid-Gas Phase Transition

$$\rho_L - \rho_G \sim (T - T_c)^{\beta}$$

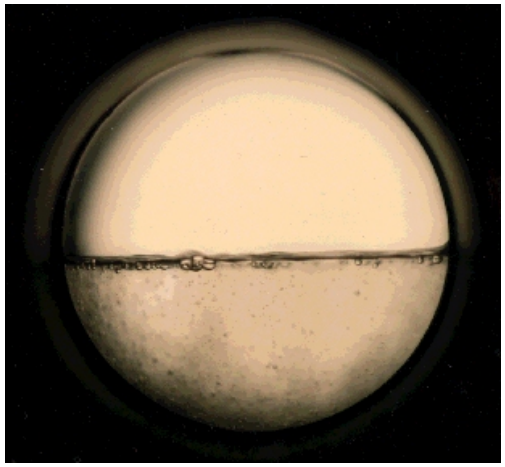
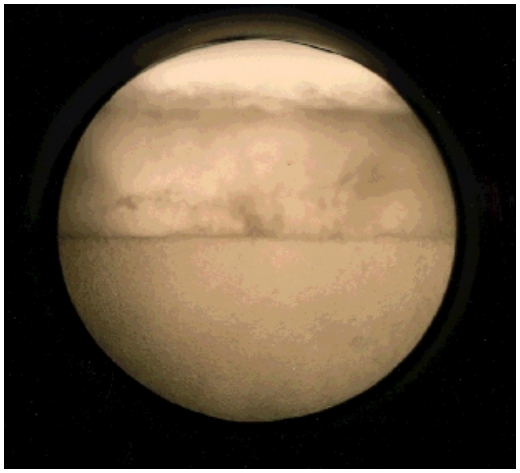
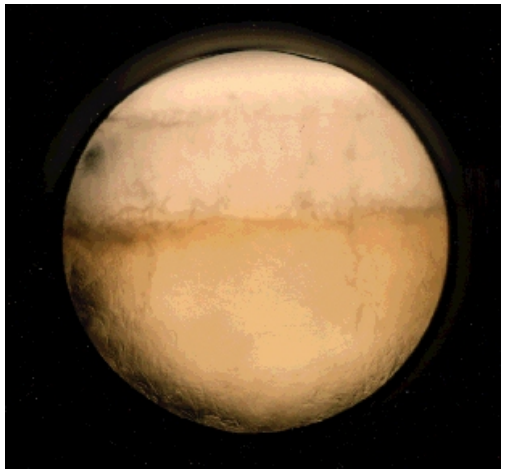
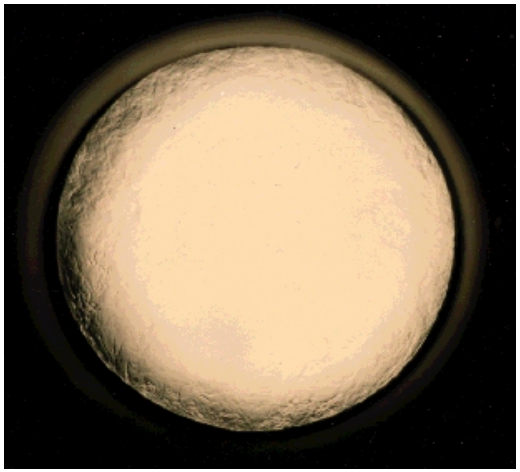
$$C_V = -T\left(\frac{\partial^2 F}{\partial T^2}\right)_V \sim |T - T_c|^{\alpha}$$



The dashed curve corresponds to the gas-liquid coexistence curve. Below the critical isotherm, the gas-liquid coexistence curve describes how large a discontinuous change in the density occurs during first-order gas-liquid phase transition. At the inflection point, which corresponds to the critical point, the discontinuity goes to 0

- The divergences in thermodynamic derivative quantities occur in the same way for systems belonging to the **same universality class**. These divergences behave as **power laws**, and hence can be described by the **exponents in the power laws**. These exponents are known as the **critical exponents**.

Critical Fluid of Carbon Dioxide

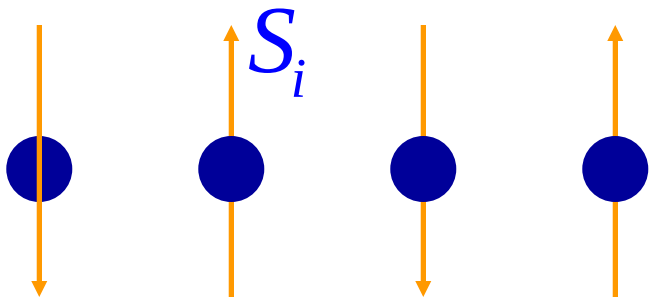





The **critical point** for carbon dioxide occurs at a pressure **p=73.8 bar** and a temperature **T_c=31.1°C**

http://www.chem.leeds.ac.uk/People/CMR/criticalvid.html

Ising Model in 1-Dimension

- The **Ising model** is a simple classical model that illustrate the physics of first and second order phase transitions, critical behavior, and hysteresis.



- the spins can point in two directions only (up or down): the up direction corresponds to spin +1 and the down direction to spin -1.
- localized spins interact with their nearest neighbors which is a model of magnetic insulator

Quantum spins → Heisenberg model

$$\hat{H} = -J \sum_{i=1}^{L-1} \hat{\vec{S}}_i \cdot \hat{\vec{S}}_{i+1}$$

$$\hat{\vec{S}}_i = \frac{\hbar}{2}\left(\hat{\sigma}_x, \hat{\sigma}_y, \hat{\sigma}_z\right)$$

Classical spins → Ising model

$$E = -J \sum_{i=1}^{L-1} S_i S_{i+1}$$

J is the exchange coupling constant

$J > 0 \Rightarrow$ energy is minimized when spins are aligned, so this models ferromagnetism

L is the number of spins

Canonical Ensemble of Statistical Physics for Systems in Contact with the Heat Bath

- The system of spins is considered to be in contact with a heat bath at temperature T.
- The set of spins can exchange energy with the heat bath, in such a way that the system can come into **thermal equilibrium** with the heat bath. In thermal equilibrium, the probability of finding the system in a particular microstate α is :

$$P_\alpha \propto e^{-E_\alpha / k_B T}$$

The right hand side of this expression is called the Boltzmann factor and k_B is the Boltzmann constant

Ising model example:

- A microstate of the system is simply a particular arrangement of spins.
- There are 2^L different possible microstates, many of which are degenerate, i.e., they have the same energy as other states.

Magnetization of Ising Ferromagnet

- Total magnetization of a particular **microstate** is:

$$M_\alpha = \sum_{i=1}^{L} S_i$$

- In general, the system does not remain in a single state but passes through many microstates which are compatible with the macrostate characterized by temperature T.
- The likelihood that it is a particular state at any time is given by P_α
- The average (or measured) values of the magnetization and energy in the **macrostate** specified by temperature T are:

$$\langle M \rangle = \sum_\alpha P_\alpha M_\alpha \qquad \langle E \rangle = \sum_\alpha P_\alpha E_\alpha$$

All Thermodynamic Quantities Can Be Obtained from the Partition Function

- Partition function is the "magic function" in Statistical Physics
- For canonical ensemble it is obtained by obtained by summing the Boltzmann factors:

$$Z = \sum_{\alpha} \exp\left(-E_{\alpha}/k_B T\right) \Rightarrow F = -k_B T \ln Z$$

- Since the probabilities must sum to unity:

$$P_{\alpha} = \frac{\exp\left(-E_{\alpha}/k_B T\right)}{Z}$$

- From Z one can compute **any other thermodynamic quantity:**

$$\frac{\partial Z}{\partial \beta} = -\sum_{\alpha} E_{\alpha} \exp\left(-\beta E_{\alpha}\right) = -Z \sum_{\gamma} E_{\alpha} P_{\alpha} = -Z \left\langle E \right\rangle$$

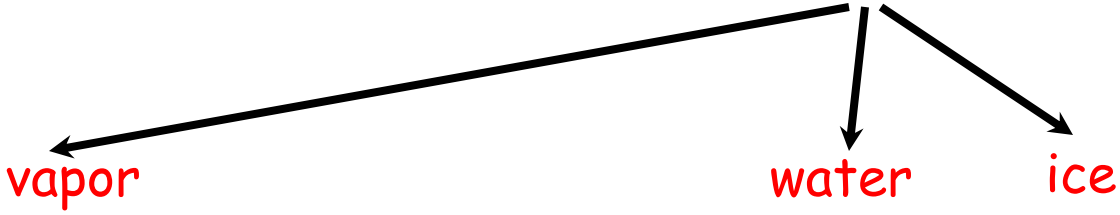
$$\Rightarrow \left\langle E \right\rangle = -\frac{\partial \ln Z}{\partial \beta}, \quad \left\langle E^2 \right\rangle = \frac{1}{Z}\frac{\partial^2 Z}{\partial \beta^2}, \quad \beta = \frac{1}{k_B T}$$

$$C_V = \frac{\partial \left\langle E \right\rangle}{\partial T} = -\frac{\beta}{T}\frac{\partial \left\langle E \right\rangle}{\partial \beta} = \frac{\beta}{T}\frac{\partial^2 \ln Z}{\partial \beta^2} = \frac{\beta}{T}\left[\frac{1}{Z}\frac{\partial^2 Z}{\partial \beta^2} - \frac{1}{Z^2}\left(\frac{\partial Z}{\partial \beta}\right)^2\right]$$

One Hamiltonian Many Phases?

- **Kramers 1936:**

$$\hat{H}\left|E_\alpha\right\rangle = E_\alpha \left|E_\alpha\right\rangle \Rightarrow Z = \sum_\alpha e^{-E_\alpha / k_B T} \Rightarrow \lim_{N\to\infty} \frac{Z}{N}$$



- As late as 1937, most of physicist were unaware of Kramer's work, and even Sommerfeld believed that the partition function describes only one phase (and could not describe liquid-gas coexistence, for example)!

- At a congress in Amsterdam to commemorate the birth of Van der Waals , there was confusion as to whether the partition function could give a sharp phase transition.

- Kramers, as chairman, put the issue to vote, but the outcome was "inconclusive"!

Brute Force Computation of the Partition Function for the Ising Model Does Not Work!

- Suppose we want to calculate the exact partition function **Z** numerically. We need to do this for all **T**, but let us start with just one temperature.

- Real system has $O(10^{23})$ spins, try first 32x32 lattice with $O(10^3)$ spins:

→Number of configurations in the sum = $2^{32\times 32} \sim 10^{300}$

→Gigantic parallel supercomputer with 10 million processors: Each processor could generate a configuration ***C***, calculate its energy **E(*C*)** and the Boltzmann factor **exp[-E(*C*)/k_BT]**, and add it to the sum over configurations in one **nanosecond**.

→The calculation runs during the whole age of the Universe:

$$10^7 \text{CPU} \times 10^9 \frac{\text{configurations}}{\text{CPU}\times\text{s}} \times 10^{14} \frac{\text{sec}}{\text{year}} 10^{10} \text{ years}$$

$$\sim 10^{40} \text{ (just for a single temperature!)}$$

Naïve Monte Carlo Numerical Sampling Does Not Work Either

- The ideal situation would be to sample configurations with a probability given by their Boltzmann weight P_α , thereby avoiding low probability microstates naïve

- The Monte Carlo Average would then be simply given by:

$$\langle M \rangle = \frac{1}{N_{MC}} \sum_{\alpha=1}^{N_{MC}} M_\alpha$$

- However, this does not work because the sampling probability:

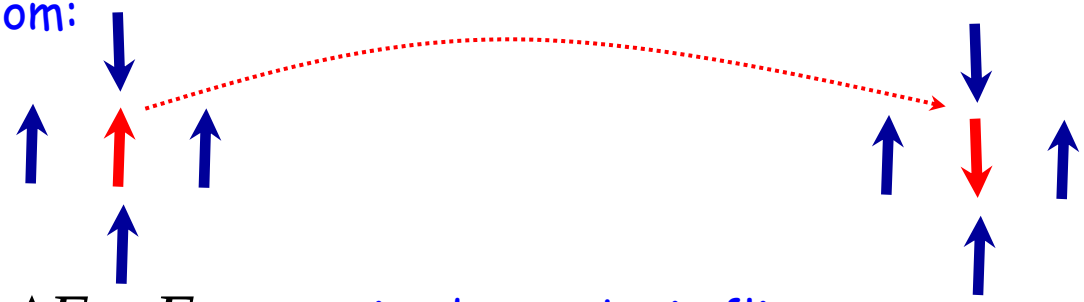
$$P_\alpha = \frac{e^{-E_\alpha / k_B T}}{Z}$$

depends on the partition function Z, which is what we are trying to calculate in the first place!

Metropolis Monte Carlo Algorithm

- The spins are initially set at random so that the starting state is paramagnetic.
- The system is then allowed to come into equilibrium with the heat bath at temperature T, using the following Metropolis Monte Carlo computational algorithm:

step 1 → Choose a spin at random:



step 2 → Calculate the energy $\Delta E = E_{flip}$ required to make it flip.

step 3

If $E_{flip} < 0$, then **flip the spin** since this will takes the system to a lower energy state.

If $E_{flip} > 0$, choose a **uniform random number** $rand \in [0,1)$

If $rand < e^{-E_{flip}/k_B T}$ then flip the spin (a processes with probability P is performed if $rand < P$). Otherwise **do not** flip the spin.

step 4 → Repeat steps 1-3 many times!

Theory Behind Metropolis Monte Carlo: Markov Chains and Detailed Balance

- Let us set up a so-called Markov chain of configurations by introducing fictitious dynamics → the "time" t is computer time (marking the number of iterations of the procedure), NOT real time since our statistical system is considered to be in equilibrium, and therefore time invariant.

→Probability to be in configuration A at time T is: $P(A,t)$

→The transition probability (per unit time) to go from A to B is: $W(A \to B)$

$$P(A,t+1) = P(A,t) + \sum_B [W(B \to A)P(B,t) - W(A \to B)P(A,t)]$$

- Equilibrium $\lim_{t\to\infty} P(A,t) = p(A)$ can be ensured by satisfying the detailed balance
- For the special case of the Boltzmann probability distribution $p(A) = e^{-E(A)/k_BT} / Z$

$$\frac{W(A \to B)}{W(B \to A)} = \frac{p(B)}{p(A)} = \frac{e^{-E(B)/k_BT}}{e^{-E(A)/k_BT}} = e^{-\Delta E/k_BT}$$

$$\Delta E = E(B) - E(A)$$

Over Los Alamos dinner party in 1953

Metropolis, Teller, and Rosenbluth chose:

$$W(A \to B) = \begin{cases} e^{-\Delta E/k_BT}, & \Delta E > 0 \\ 1, & \Delta E \le 0 \end{cases}$$

General Requirements for Validity of Monte Carlo Algorithms

- **Valid Monte Carlo algorithm requires that:**

1. We have a means of generating a new configuration **B** from a previous configuration **A** such that the transition probability $W(A \rightarrow B)$ satisfies detailed balance.

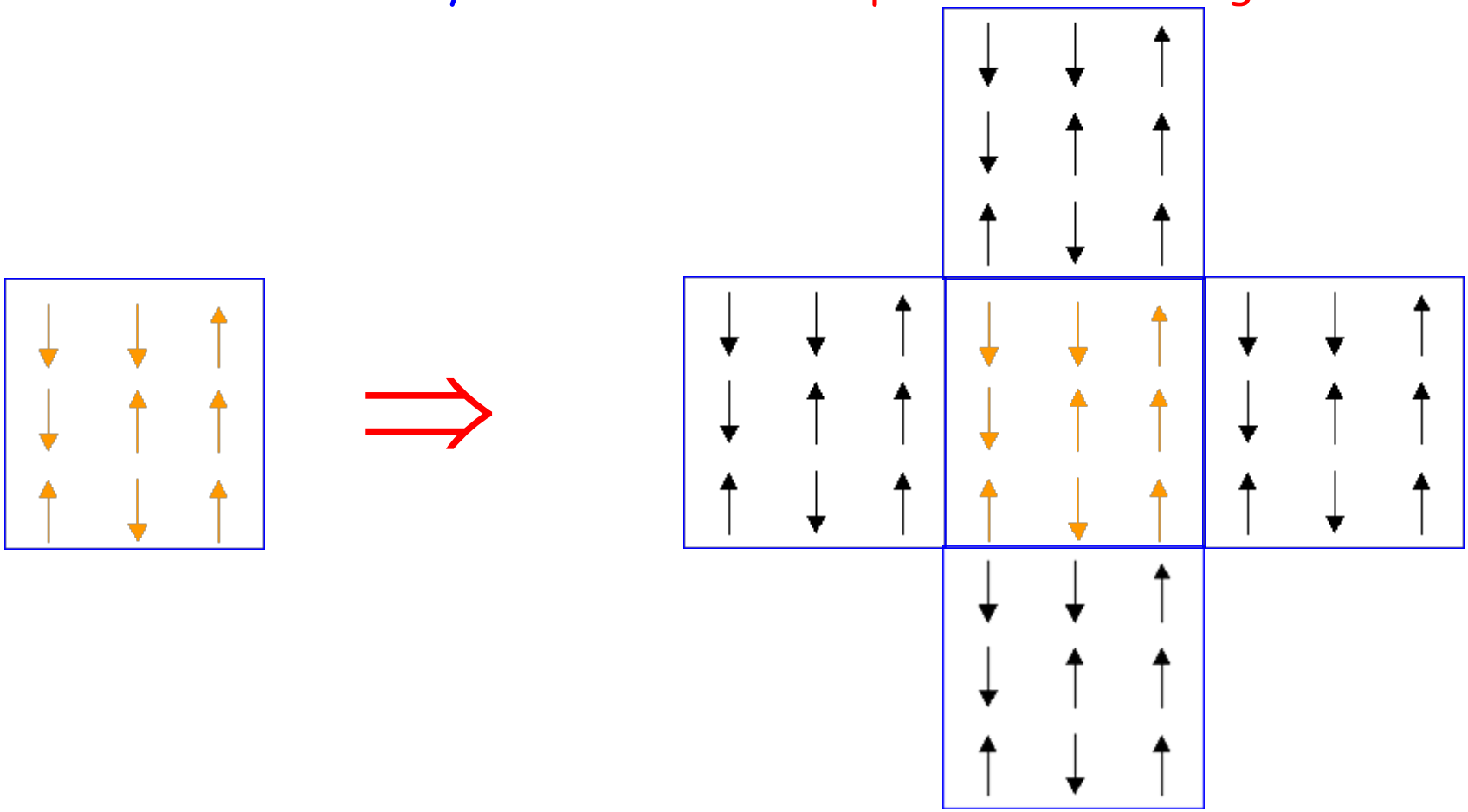
2. The generation procedure is **ergodic**, so that every configuration can be reached from every other configuration in a finite number of iterations.

- **Metropolis** algorithm satisfies the first criterion for all statistical systems.

- Second criterion is model dependent, and not always true (e.g. at **T=0**).

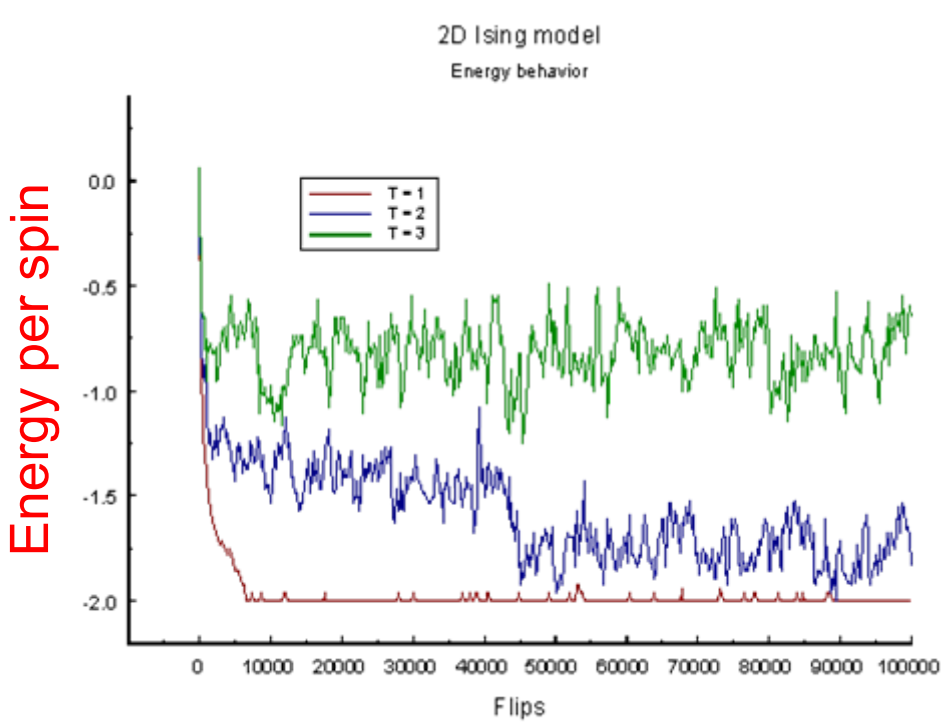
Remove Edge Effects by Using Periodic Boundary Conditions

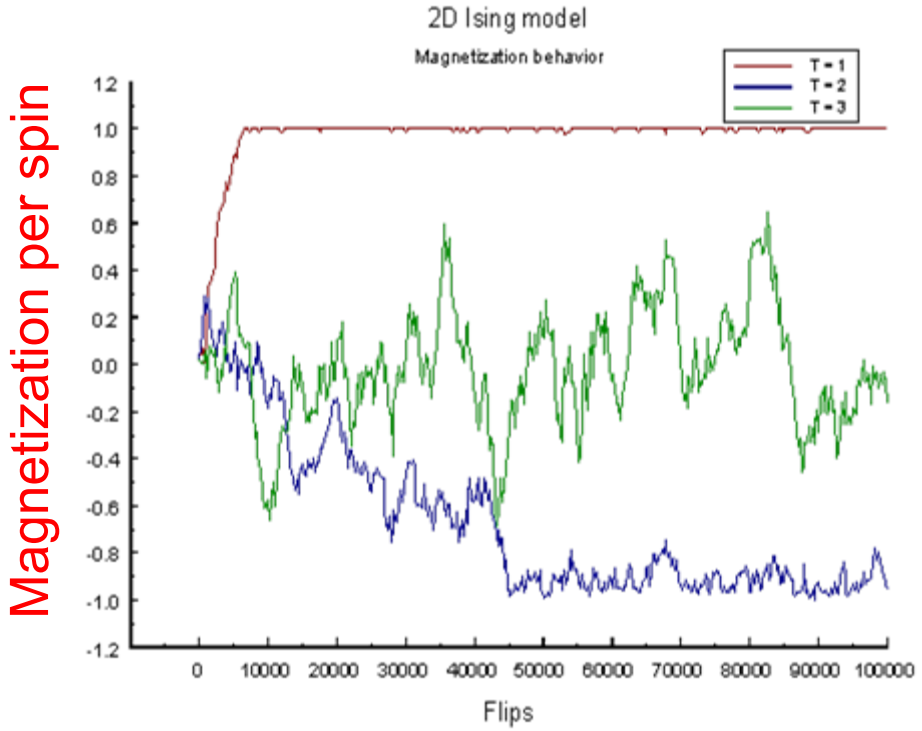
- Spins are arranged on a square grid, with L spins on a side.
- To reduce the effects of the edges and focus on the bulk properties introduce Periodic Boundary Conditions: each spin now has 4 neighbors.



Fluctuations in Monte Carlo Time "Evolution"

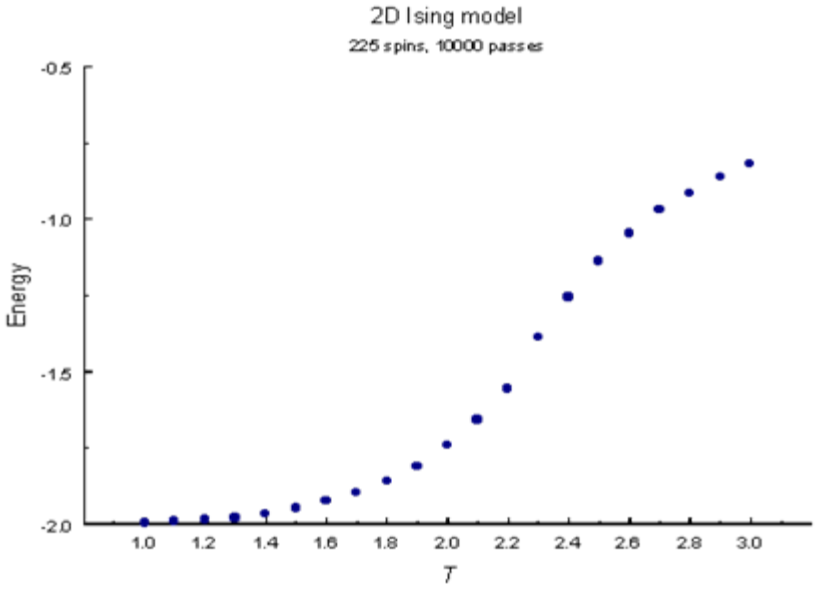
- After sufficient MC "time" steps, the system comes into equilibrium with the heat bath. There will be fluctuations in E and M but the mean rate of energy increasing transitions will become the same as the mean rate of energy decreasing transitions.

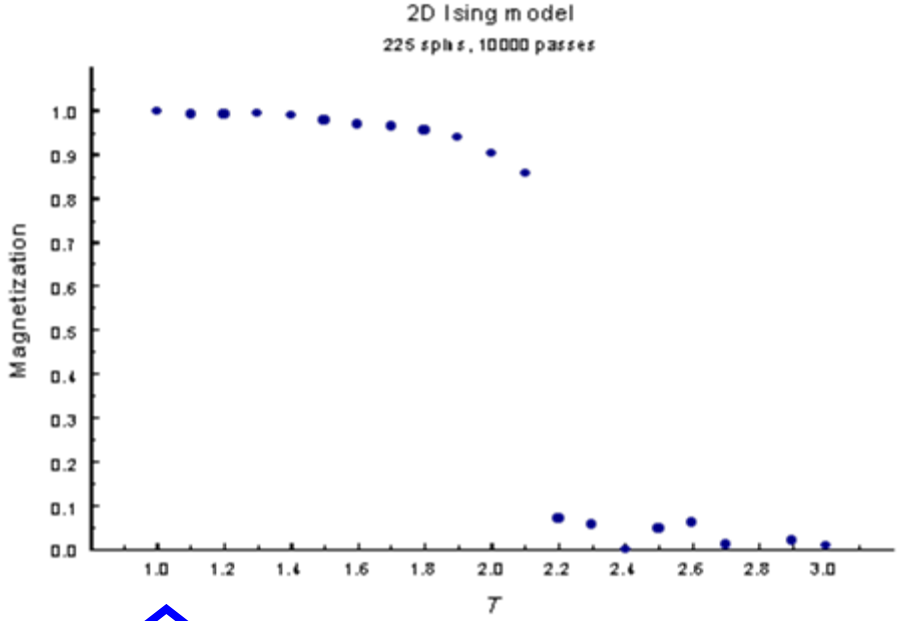


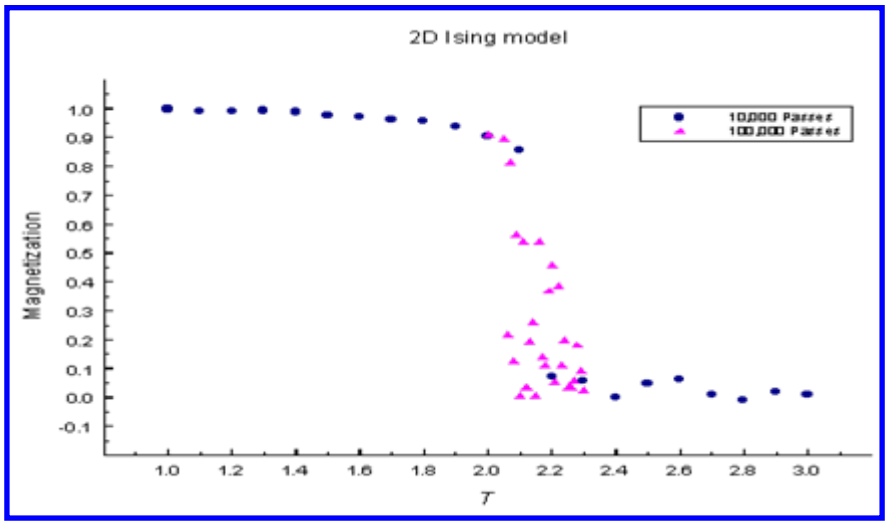


- The higher the temperature the higher the energy. At low temperatures the spins arrange themselves into a ferromagnetic state. At high temperatures, the mean magnetization is zero, i.e., the system is paramagnetic.

Energy and Magnetization vs. Temperature







Add more points around the critical temperature to fill the gap!

Fluctuation-Dissipation Theorem Gives Expressions for the Response Functions

- Response functions (and, therefore, dissipation) are related to fluctuations in equilibrium:

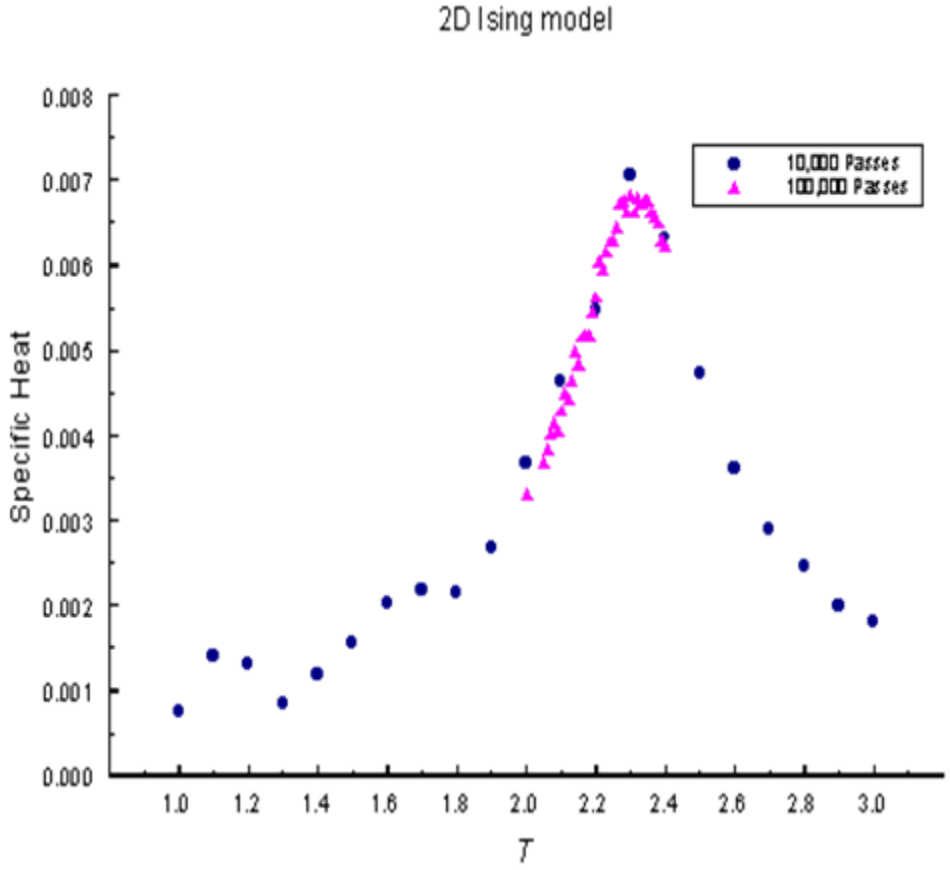
$$C_V \overset{def}{=} \frac{\partial \langle E \rangle}{\partial T} \Leftrightarrow C_V = \frac{\beta}{T}\left[\langle E^2 \rangle - \langle E \rangle^2\right] = \frac{(\Delta E)^2}{k_B T^2}$$

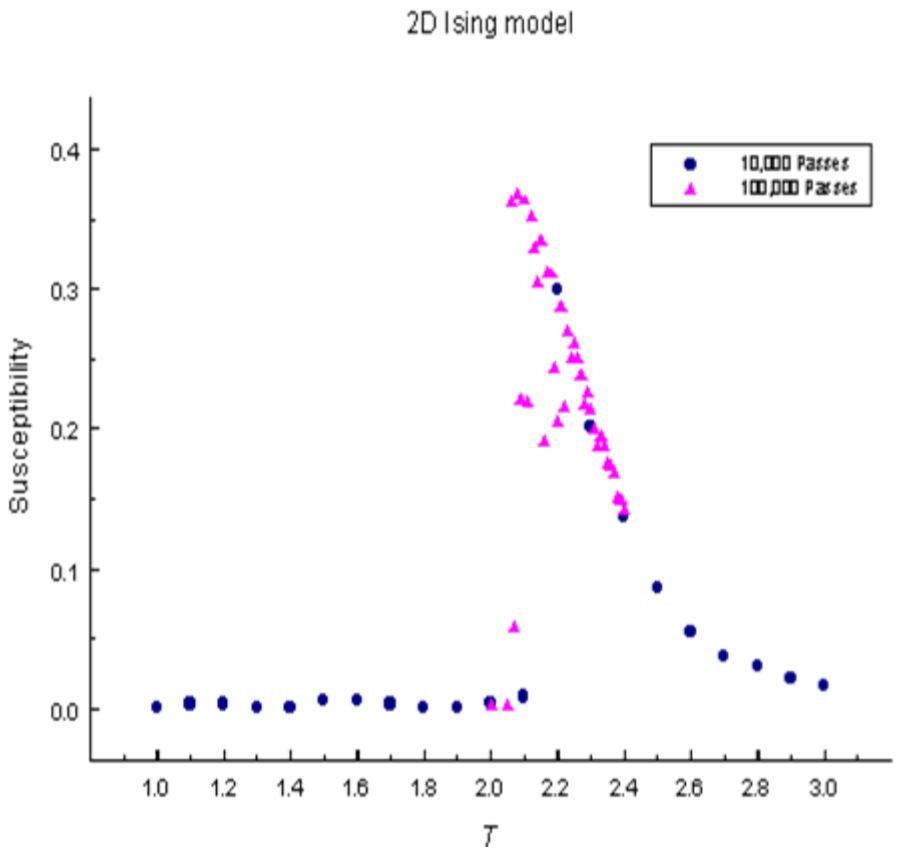
$$\chi \overset{def}{=} \frac{\partial \langle M \rangle}{\partial H} \Leftrightarrow \chi = \beta\left[\langle M^2 \rangle - \langle M \rangle^2\right]$$

- We expect that specific heat per spin does not depend on the total system size. Therefore fluctuations become less important in large systems (true away from critical points!):

$$\frac{C_V}{L} = \frac{\beta}{T}\frac{(\Delta E)^2}{L} \neq f(L) \Rightarrow \frac{\Delta E}{E} \propto \frac{1}{\sqrt{L}} \underset{L\to\infty}{\to} 0$$

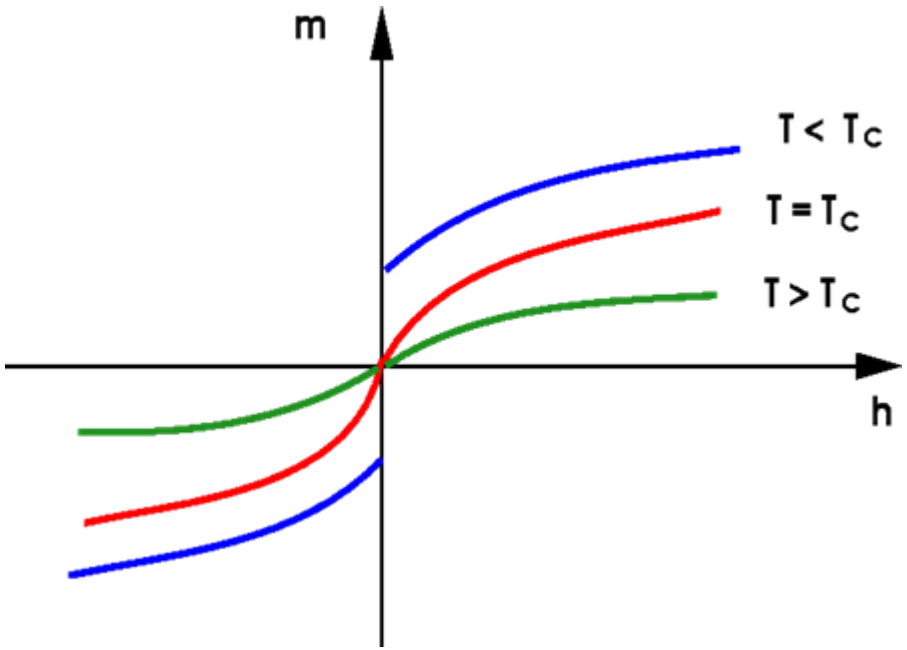
Singular (!) Physical Quantities Near the Critical Point

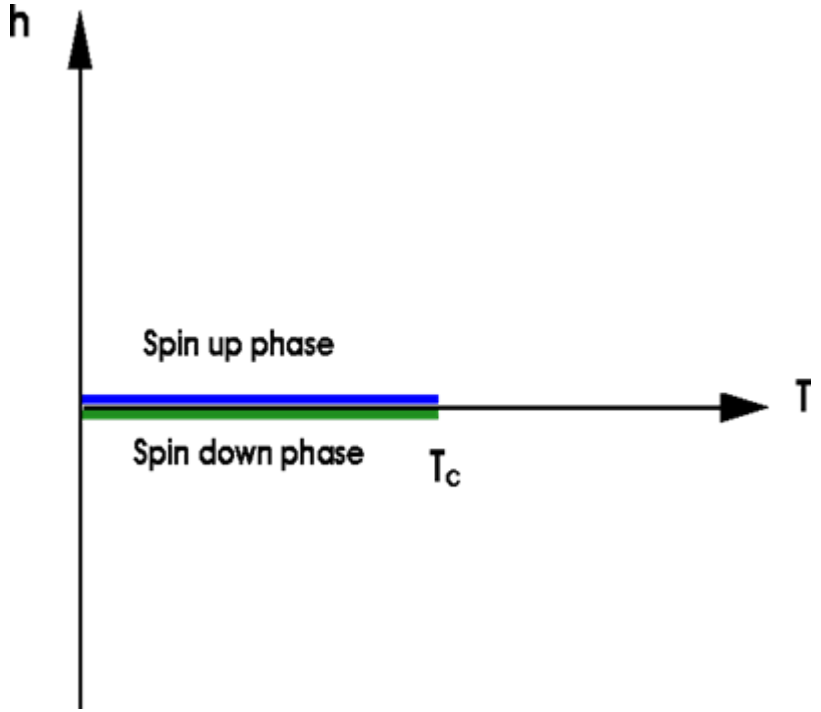




- The differences between the Monte Carlo simulation and the exact analytical results (when they exist) arise primarily from using a **finite number of spins in computer simulations**.

First and Second Order Phase Transitions in Ferromagnet-Paramagnet Systems





- Notice an inflection point along the isotherm:

$$\frac{\partial m}{\partial h} \to \infty, T = T_c \text{ and } h = 0$$

$$m \sim (T_c - T)^{\beta}, T < T_c$$

All Divergences at T_c Can Be Reduced to Fundamental Divergence of the Correlation Length

- Order parameter – **magnetization** – can be written as the volume integral over the magnetization density:

$$M = \left\langle \int d\mathbf{r} m(\mathbf{r}) \right\rangle, \quad \langle \ldots \rangle = \frac{1}{Z} \int \ldots e^{-\beta H}$$

- Correlation function:

$$\Gamma(\mathbf{r}) = \langle m(\mathbf{r}) m(0) \rangle - \langle m(\mathbf{r}) \rangle \langle m(0) \rangle = \left\langle \left(m(\mathbf{r}) - \langle m(\mathbf{r}) \rangle \right) \left(m(0) - \langle m(0) \rangle \right) \right\rangle$$

shows how the value of the order parameter at one point is correlated to its value at some other point.

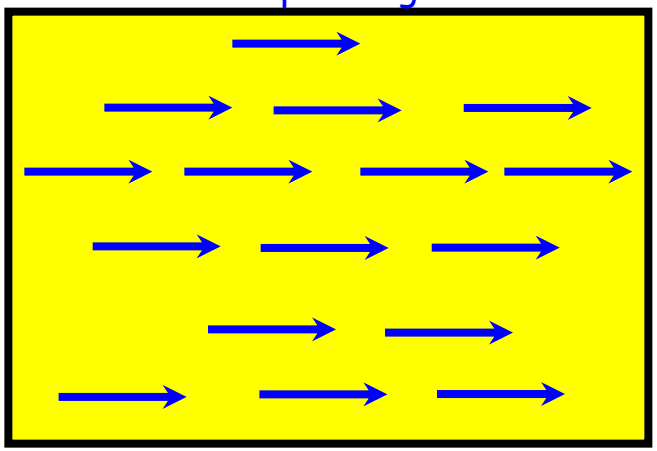
- If decreases very fast with distance, then far away points are relatively uncorrelated and the system is dominated by its microscopic structure and short-ranged forces.
- A slow decrease would imply that faraway points have a large degree of correlation or influence on each other.
- The system thus becomes organized at a macroscopic level with the possibility of new structure beyond the obvious one dictated by the short-ranged microscopic forces:

$$T \to T_c \Rightarrow \Gamma(\mathbf{r}) = r^{-p} e^{-r/\xi}$$

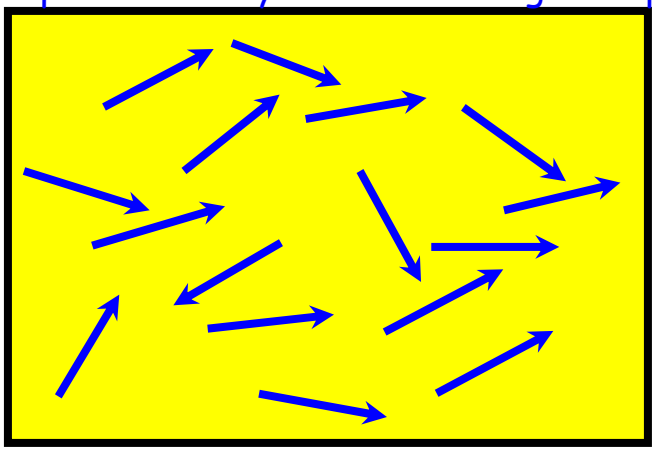
$$\text{at } T_c : \xi \sim \left| \frac{T - T_c}{T_c} \right|^{-\nu}, \Gamma(\mathbf{r}) = r^{-p}, p = d - 2 + \eta$$

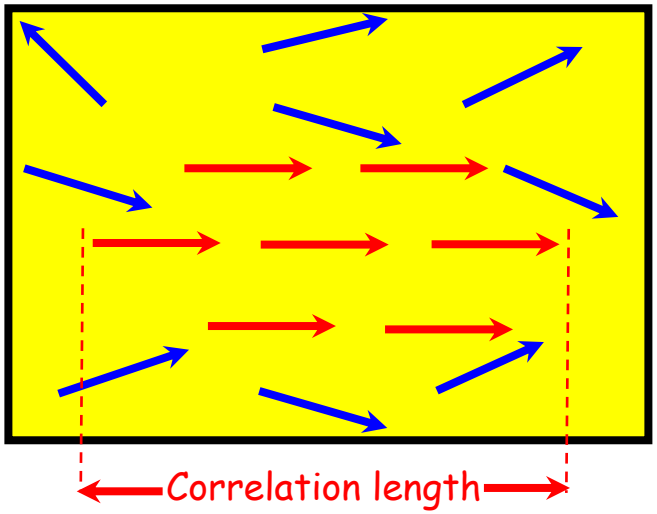
Correlation Length in Pictures

All lattice spins aligned at T=0



Lattice spins randomly oriented at high temperature





Correlated groups of spins as the critical temperature is approached from above

Critical Slowing Down

- Ising model does not have dynamics built into it - there is no kinetic energy term associated with spins – so that Metropolis Monte Carlo method generated successive configurations of spins do not represent the real time evolution. Nevertheless, it is useful to measure a relaxation time for the "Metropolis dynamics" because it helps to determine how many steps to discard in order to generate statistically independent configurations:

$$C(\tau) = \frac{1}{N-\tau}\sum_{t=0}^{t-\tau-1} M_t M_{t+\tau} \sim e^{-t/\tau}$$

$$\tau \sim \xi^z \sim |T - T_c|^{\nu z}$$

$$z \simeq 2.1$$

- The maximum possible value for ξ in system of $N = L \times L$ spins is $\xi \sim L$, so that $\tau \sim L^{2.1} \sim N$ around T_c .
- This makes simulations difficult because the Metropolis algorithm time scales like N, so the time to generate independent Metropolis configurations scales like $N\tau \sim N^2 = L^4$.
- Metropolis algorithm is a local algorithm where one spin is tested and flipped at a time. Near T_c the system develops large domains of correlated spins which are difficult to break up -> use non-local or cluster algorithms (such as Wolf algorithm).