Programming Seminar: 4. Ising Model

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Introduction

The Ising model is one of the firsts attempts to the phase transitions theory.

Thermodynamics and Phase Space

On Thermodynamics and Statistical Mechanics there are two different meanings for *phase space*

Classical Mechanics Phase Space:	Thermodynamics Phase Space:
Has the information of the Micro-State of the system.	Has the information of the Macro-State of the system.
Coordinates and canonical momenta	For instance PVT

During this presentation we'll refer as phase space the thermodynamical phase space.

Phase Transitions

The phase transitions are understood as changes on macroscopic behavior given a external stimulus.

Typically changes from liquid to solid or gas are studied.

We're going to focus on a magnetic system.

Critical Behavior

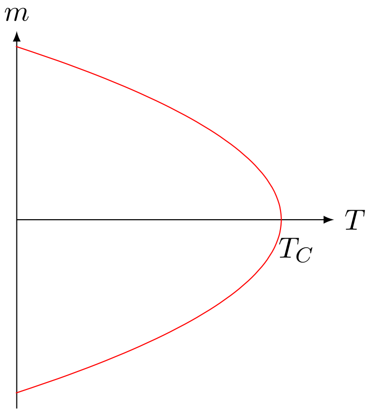

Figure 1: Singular behavior

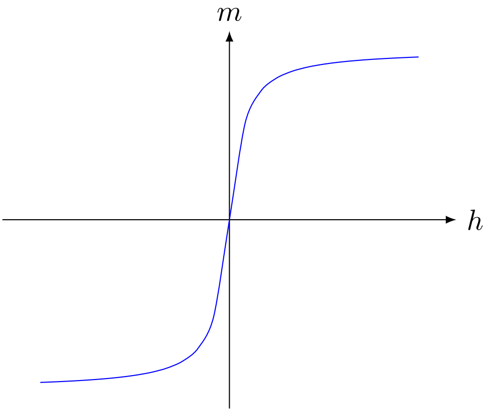

Figure 2: Singular behavior

Order Parameter

Order Parameter

Is a thermodynamic function that can be used to distinguish between phases.

For a magnet system the *magnetization* can be used as parameter

$$m(T) = \frac{1}{V} \lim_{h \longrightarrow 0} M(h, T) \tag{1}$$

Critical Exponents

The behavior of the order parameter near the transition is given by a critical exponent.

$$m(T = T_c, h) \propto h^{1/\delta} \tag{2}$$

or

$$m(T, h = 0) \propto \begin{cases} 0 & \text{for} \quad T > T_c \\ |t|^{\beta} & \text{for} \quad T < T_c \end{cases} \tag{3}$$

Response Functions

Near the critical point, the system is very sensitive to external perturbations.
In the case of magnetization the response field is the magnetic susceptibility

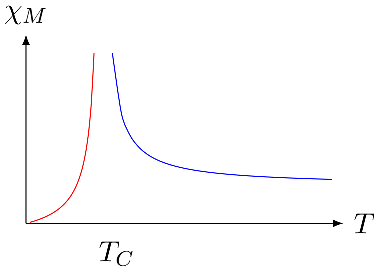

Figure 3: Different behaviors near the transition point.

Long-Range Correlations

Macroscopic Response Functions $\longleftrightarrow$ Microscopic Fluctuations

The partition function of a magnetic system in a magnetic field h is given by

$$Z(h) = \mathrm{Tr}\left\{\exp[-\beta\mathcal{H}_0 + \beta h M]\right\} \tag{4}$$

Where $\mathcal{H}_0$ is the energy of the magnet, and $-hM$ is the work done against the magnetic field.

Using that the average of an observable is calculated as

$$\langle A \rangle = \frac{1}{Z} \operatorname{Tr} \{ A \exp[-\beta \mathcal{H}_0 + \beta h M] \} \tag{5}$$

The average of the magnetization

$$\langle M \rangle = \frac{\partial \ln Z}{\partial (\beta h)} = \frac{1}{Z} \operatorname{Tr} \{ M \exp[-\beta \mathcal{H}_0 + \beta h M] \} \tag{6}$$

And the susceptibility as the variance

Relation with the Correlation Function

The total magnetization is given as

$$M = \int d\mathbf{r} m(\mathbf{r}) \tag{7}$$

so,

$$\chi_M = \int d\mathbf{r} \int d\mathbf{r}' \left(\langle m(\mathbf{r}) m(\mathbf{r}') \rangle - \langle m(\mathbf{r}) \rangle \langle m(\mathbf{r}') \rangle \right) \tag{8}$$

Now, we get

- $\langle m(\mathbf{r}) \rangle = m$
- $\langle m(\mathbf{r}) m(\mathbf{r}') \rangle = G(\mathbf{r} - \mathbf{r}')$

Ising Model

The Ising model is the simplest model to explain magnetism. Proposed by Ising on his doctoral thesis.

It is based on having fixed spins on a lattice that can only take values of 1 or -1

$$\mathcal{H} = -\sum_{\langle i,j \rangle} J_{i,j} \mathbf{s}_i \cdot \mathbf{s}_j \tag{9}$$

where $J_{i,j}$ is the exchange energy of the interaction and $\mathbf{s}_{i,j}$ are the spins on the position i and j respectively.

The summation is done only counting the neighbours.

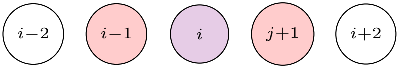

Figure 4: One Dimensional Example

The interactions are local, the purple only *feels* the interaction with the red ones.

Statistical Mechanics

We are going to use a statistical mechanics approach.

Which ensemble is the correct one?

We may consider initially

- Micro-Canonical: Isolated.
- Canonical: Thermal equilibrium with environment.
- Grand-Canonical: Thermal and chemical equilibrium with environment.

The correct one is the Canonical!

Temperature on the Model

One of the biggest questions until this point is.

How do we introduce the temperature?

A://The numerical method.

Metropolis Algorithm

The Metropolis algorithm is based on which configuration is more probable.

In our context it can be thought as the *more energetic favourable* configuration.

And is in this point where the canonical ensemble takes place.

Implementation

The implementation is straightforward

- Choose a position on the lattice.
- Generate a possible new value.
- Calculate the difference of the energy $\Delta E = E_{\text{old}} - E_{\text{new}}$.
  - If $\Delta E < 0$: replace the old value.
  - If $\Delta E > 0$: Compare with the canonical probability.

$$p(E) = \exp\left(-\frac{\Delta E}{k_B T}\right)$$

  - Else, reject the E_{new} configuration.
- Repeat until *stabilization*

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