Complex Systems Methods — 7. Critical Phenomena: Phase transition, Ising model

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Overview

1. Introduction
   - Critical Phenomena
   - Phase transitions
   - Landau theory
   - Scaling and critical exponents
2. Statistical Mechanics
   - Micro— and Macrostates
   - Statistical ensembles as maximum entropy distributions
   - Continous phase transitions in statistical physics
   - The Ising Model

What are critical phenomena?

- Critical phenomena occur in critical states.
- A system is in a critical state, if it is extremely susceptible to small perturbations. More formally: divergence of susceptibilities.
- High probability of ,,extreme events" — critical fluctuations (response and fluctuations are related by dissipation-fluctuation theorems)
- Properties of critical states: *self similarity*, no typical length and/or time scales $\longrightarrow$ power law correlations $\longrightarrow$ long-range or long-term correlations, respectively.
- Slowly decaying correlations $\Rightarrow$ Criticality as paradigm for complexity.
- Critical states are observed at continous phase transitions

Phase transitions

1. Heterogeneous systems: qualitative changes of macroscopic properties at boundary layers $\Rightarrow$ the hommogenous parts are called *phases*
2. Qualitative change of macroscopic properties of a homogeneous system due to a changing *control parameter* $\Rightarrow$ *phase transition*
3. Usually a phase transition is related to a change in the degree of order in the system quantified by the *order parameter* —- spontaneous symmetry breaking
4. Examples:
   - solid-fluid-gaseous
   - Magnetic phase transitions: Ferro- and antiferromagnetic
   - Structural phase transitions
   - Macroscopic quantum phenomena: superconductivity, suprafluiditiy, Bose-Einstein condensation
   - ...

Thermodynamic potentials

- Scalar function of the state variables (control variables) of the system. which represents the state of the system, depndent variables as derivations
- First law of thermodynamics $dU = \delta Q - \delta W$.
  With the entropy $dS = \frac{\delta Q}{T}$ and the mechanical work pdV we get

$$dU = TdS - pdV$$

  i.e. the internal energy U as a thermodynamic potential $U(S, V)$ for the state variables entropy S and volume V.
- For a gas the state variables are volume V and temperature T leading to the free energy

$$F = U(V, T) - TS(V, T) \qquad dF = -pdV - SdT$$

Conjugated variables - First derivatives

- Using pressure p and temperature T leading to the free enthalpy (Gibbs free energy)

$$G = U(p,T) + pV(p,T) - TS(p,T) \qquad dG = -SdT + Vdp$$

- Conjugated variables

$$S = -\left(\frac{\partial F}{\partial T}\right)_V \qquad p = -\left(\frac{\partial F}{\partial V}\right)_T$$
$$S = -\left(\frac{\partial G}{\partial T}\right)_p \qquad V = \left(\frac{\partial G}{\partial p}\right)_T$$

Response functions - Second derivatives

- Response functions quantify the response of the system with respect to a changing control parameter or external field, respectively
- Specific heat

$$C_V = \left(\frac{\partial Q}{\partial T}\right)_V = T\left(\frac{\partial S}{\partial T}\right)_V = -T\left(\frac{\partial^2 F}{\partial T^2}\right)_V$$

- Kompressibility

$$\kappa_T = -\frac{1}{V}\left(\frac{\partial V}{\partial p}\right)_T = -\frac{1}{V}\left(\frac{\partial^2 G}{\partial^2 p}\right)_T$$

- Magnetic susceptibility

$$\chi_T = \frac{1}{\mu_0}\left(\frac{\partial M}{\partial H}\right)_T = -\frac{1}{\mu_0}\left(\frac{\partial^2 G}{\partial^2 H}\right)_T$$

First- and second order phase transitions

- Phase transitions related to singularities in the thermodynamic potential
- Phase transition of n-th order: Discontinouity in the n-th derivation of the thermodynamic potential
- First order: discontinuity in the conjugated variables — discontinuity in the order parameter
- Second order: discontinuity in the suceptibilities, e.g. specific heat or magnetic suceptibility

Landau theory — Phenomenological theory of phase transitions

- Gibbs free energy of the ferromagnet as function of the temperature T and the external field H:

$$G(T, H, M_{eq}(H, T)) = U - MH - TS \qquad dG = -MdH - SdT$$

- Landau theory: phenomenological ansatz for the Gibbs free energy (constrained equilibrium)

$$G(T, M, H) = -MH + G(T, M, 0)$$

- Equilibrium:

$$\left(\frac{\partial G}{\partial M}\right)_{H,T} = 0 \qquad \left(\frac{\partial^2 G}{\partial M^2}\right)_{(H,T)} > 0$$

- Expansion around the equilibrium point:

$$G(T, M, 0) = G_0(T) + \frac{a(T)}{2} M^2 + \frac{b(T)}{4} M^4$$

Landau theory

- Equilibrium for $H = 0$: $\partial G_0/\partial M|_T = 0$
  $\Rightarrow M = 0$ or $M^2 = -a(T)/b(T)$.
- In order to get a phase transition: $a(T) = \frac{T-T_c}{c} + \dots$
- $M \propto -(T - T_c)^{1/2}$
- $H \neq 0$:

$$G(T, M, H) = G_0(T) + \frac{T - T_c}{2c} M^2 + \frac{b}{4} M^4 - HM$$

- Magnetization:

$$H = \frac{T - T_c}{c} M + bM^3 \quad T = T_c : M \propto H^{1/3}$$

- Susceptibility:

$$
\begin{aligned}
\chi_T &= \frac{1}{\mu_0}\left(\frac{\partial M}{\partial H}\right)_{T,H=0} \\
&= \frac{1}{\mu_0}\frac{1}{\left(\frac{\partial H}{\partial M}\right)_{T,H=0}} \\
&= \frac{1}{\mu_0}\frac{1}{\frac{T-T_c}{c}+3bM^2} \\
&= \begin{cases} \frac{c}{\mu_0(T-T_c)} & T > T_C \\ \frac{c}{2\mu_0(T_c-T)} & T < T_c \end{cases}
\end{aligned}
$$

Critical exponents

- Empirical observation: power law behaviour near the phase transition

$$\epsilon = \frac{T - T_c}{T}$$

- Specific heat $c_V \propto \epsilon^{-\alpha}$ for $\epsilon > 0$, $c_V \propto (-\epsilon)^{-\alpha'}$
- Order parameter: $M \propto (-\epsilon)^{\beta}$
- Order parameter and external field at the phase transition $T = T_c$

$$M \propto H^{1/\delta}$$

- Susceptibility $\chi_T \propto \epsilon^{-\gamma}$, $\chi_T \propto (-\epsilon)^{-\gamma'}$
- Correlation function $\langle \delta M(r + r')\delta M(r) \rangle \propto e^{-r'/\xi}$, $\xi \propto \epsilon^{-\nu}$
- Landau theory: $\alpha = \alpha' = 0$,$\beta = 1/2$,$\gamma = \gamma' = 1$ and $\delta = 3$.

Scaling hypothesis

- Kadanoff 1967: The singular part of the thermodynamic potential is a homogeneous function

$$G_S(\lambda^{a_\epsilon}\epsilon, \lambda^{a_H}H) = \lambda G_S(\epsilon, H)$$

- ϵ-scaling: $\lambda = |\epsilon|^{-1/a_\epsilon}$

$$G_S(\epsilon, H) = |\epsilon|^{1/a_\epsilon} G_S(\pm 1, |\epsilon|^{\frac{a_H}{a_\epsilon}} H)$$

- Critical exponents can be expressed by a_H and a_ϵ, e.g.

$$M = -\left(\frac{\partial G_S}{\partial H}\right)_{H=0} \Rightarrow \beta = \frac{1 - a_H}{a_\epsilon}$$

- a_ϵ and a_H are phenomenological parameters, but can be determined by a microscopic theory $\Rightarrow$ renormalization group

Micro— and Macrostates

- Classical thermodynamics worked with macroscopic observables: volume, pressure, temperature, entropy...
- If the systems consist of particles, the state of the system is given by microscopic observables: position, velocity
- Statistical mechanics: Explaining the macroscopic properties from microscopic laws
- Maximum entropy principle: A macrostate is described by a distribution over microstates where the values of the macroscopic observables are given by the expectectation values and which has besides maximum entropy, i.e. it contains no additional information about the system.
- Energy constant: uniform distribution on the energy hyperplane — microcanocical distribution

Ensembles from the maximum entropy principle

System described by a set of macroscopic observables $\{A_i\}$ with values $\hat{A}_i$, which are functions of the microscopic state variables $\boldsymbol{x}$. We are looking for a distribution $p(\boldsymbol{x})$ with

$$\hat{A}_i = \langle A_i \rangle = \int d\boldsymbol{x} p(\boldsymbol{x}) A_i(\boldsymbol{x})$$

and

$$S = -\int d\boldsymbol{x} p(\boldsymbol{x}) \log p(\boldsymbol{x}) - \sum_i \lambda_i (\hat{A}_i - \langle A_i \rangle) \stackrel{!}{=} \text{Maximum}$$

with $A_1 = 1$ for the normalization.

Maximum entropy distributions

$$
\begin{aligned}
P(\boldsymbol{x}) &= \frac{1}{Z}\exp\left[-\sum_{i=1}^{m}\lambda_i A_i(\boldsymbol{x})\right] \\
\langle A_i\rangle &= -\frac{\partial \ln Z}{\partial \lambda_i} \\
Z &= \int d\boldsymbol{x}\exp\left[-\sum_{i=1}^{m}\lambda_i A_i(\boldsymbol{x})\right]
\end{aligned}
$$

- Entropy:

$$S = k\sum_i \lambda_i\langle A_i\rangle + k\ln Z$$

- Only $A_2 = \langle E\rangle \Rightarrow \lambda_2 = \beta = 1/kT \Rightarrow$ canonical ensemble

Phase transitions

Partition function becomes singular, but only in the thermodynamic limit $V, N \to \infty$, $N/V = const$. For finite systems there is a non-zero probability to change the phase.

The Ising model

- Binary variables (spins, magnetic moments) s_i on a lattice
- Pairwise interactions with energy $-J_{ij}s_j s_i$. Energy $E = -\sum_i(\sum_j J_{ij}s_i s_j + Hs_i)$ with the external field H. Canonical distribution
$$p(s_1, \ldots, s_N) = \frac{1}{Z}e^{\beta \sum_i(\sum_j J_{ij}s_i s_j + Hs_i)}$$
- Paradigmatic model for a second order phase transition.
- Simplified model to describe the ferromagnetic phase transition.
- J_{ij} random - spin glasses
- Many applications in a large variety of fields:
  - Phase separation
  - Opinion dynamics
  - Segregation
  - Memory, pattern recognition (Hopfield network)
- Extensions: more states of the local variable — Potts model

The Phase transition in the mean field approximation

- Energy can be written as $E = -\sum_i s_i(\sum_j J_{ij}s_j + H)$.
- Approximating the local field by a mean field

$$(\sum_j J_{ij}s_j + H) \approx J_0\langle s\rangle + H = \bar{H}$$

with $J_0 = \sum_j J_{ij}$.

- $\Rightarrow$ effective one particle Hamiltonian

$$p_{mf}(s_1, \ldots, s_N) = \frac{1}{Z}\prod_i \exp(-\beta s_i \bar{H})$$

and

$$Z = Z_i^N \qquad Z_i = 2\cosh\beta\bar{H}\ .$$

Properties of the mean field solution

- Solution: self-consistent solution of the mean field equation

$$\begin{aligned}\langle s\rangle &= \sum_{s_i} s_i \frac{\exp(-\beta s_i \bar{H})}{Z_i} \\ &= \frac{1}{2}\tanh\beta\left(J_0\langle s\rangle + H\right)\end{aligned}$$

- Critical exponents in the mean field solution the same as in the Landau theory: $\beta = 1/2$, $\gamma = 1$,$\delta = 3$.
- $\Rightarrow$ Landau theory corresponds to a mean field approximation

Exact solutions of the Ising model on a square lattice

- Exact solution for the 1-D Ising model: no phase transition, correlation length diverges at $T = 0$.
- Onsager 1944 published an exact solution for the 2-D Ising model with nearest neighbour interactions on a square lattice.
- Critical temperature: $sinh^2 2\frac{J}{kT_c} = 1$
- Specific heat diverges logarithmically $C \propto \ln |T - T_c|$
- Magnetization $M \propto (T_c - T)^{1/8}$

	C, α	M, β	χ, γ	M, δ	ξ, ν
Mean field	0	1/2	1	3	
2-D Ising	0 (ln)	1/8	7/4	15	1
3-D Ising	≈ 0.1	$\approx 5/16$	$\approx 5/4$	≈ 5.05	≈ 0.638

Excess entropy of Ising model on a square lattice

Erb/Ay, J.Stat.Phys. 115(2004),949

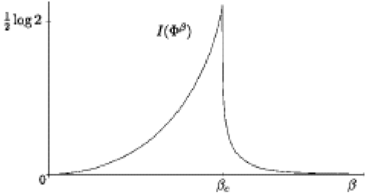

Fig. 4. Multi-information of the Ising square lattice.

- Exact result for the entropy of the 2-D Ising model allows to calculate the multi-information (integration) $I = \sum_i H(s_i) - H(s_1, \ldots, s_N)$. Multi-information becomes maximal at T_c.
- 1-D Ising model is Markov chain - both excess entropy and multi-information per spin agree and become maximal for $T \rightarrow 0$.