Complex Systems Methods — 8. Critical Phenomena: Ising model, Renormalization

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Potsdam WS 2007/08

Overview

1. Exact results for the Ising model
   - Exact solution of the 1-D Ising model
   - High- and low temperature expansion
   - The dual lattice
   - Transfer matrix method
2. Scaling, Renormalization and Universality
   - Stable Distributions
   - Period doubling transition to chaos

Open questions from last lecture

1. Why are spin glasses called "glasses" and how is the "glassy" state defined thermodynamically?
    - Glasses are supercooled *frozen* liquids
    - Extremely long relaxation times
    - Metastable states
2. What are the controversies about Jaynes maximum entropy principle?
    - Basically the controversy between frequentist and Bayesian, between objective and subjective probabilities
    - For instance entropy: in which sense can it be an objective "physical" property, if it does only reflect our knowledge about the system?
3. What can we really learn about the nature of temperature from the maximum entropy approach?
    - (Inverse) temperature in the form of the Lagrange multiplier β has to be determined from

$$\hat{E} = \langle E \rangle = -\frac{\partial \ln Z}{\partial \beta}$$

Not a deep insight !?

Ising Model

- Schematic model for the ferromagnetic phase transition
- Binary spin variable $s_i = \{-1, 1\}$.
- In the following we assume next neighbour interaction.
  To produce one pair of non-aligned neighbouring spins one needs energy J, i.e.

$$E = -\sum_{\langle ij \rangle} \frac{J}{2} s_i s_j - s_i H$$

  with $\langle ij \rangle$ denoting pairs of adjacent spins i, j.
- We have the partition function

$$Z = \sum_{s_1, s_N} e^{\beta\left(\sum_{\langle ij \rangle} \frac{J}{2} s_i s_j - s_i H\right)}$$

- Gibbs free energy $G = -\frac{1}{\beta} \ln Z$
- the magnetization $M = -\frac{1}{\beta} \frac{\partial \ln Z}{\partial H}$ and
- the magnetic susceptibility $\chi = -\frac{1}{\mu_0 \beta} \frac{\partial^2 \ln Z}{\partial H^2}$

Excat results — The partition function

- Nearest neighbour interaction with strength $J/2$.
- Abbreviation:

$$L = \frac{\beta J}{2}$$

- Partition function

$$Z = \sum_{s_1=\pm 1} \dots \sum_{s_N=\pm 1} \prod_{\langle ij \rangle} \exp(L s_i s_j)$$

- The identity

$$\exp(L s_i s_j) = \cosh L + s_i s_j \sinh L$$

leads to

$$Z = \sum_{s_1=\pm 1} \dots \sum_{s_N=\pm 1} \prod_{\langle ij \rangle} (\cosh L + s_i s_j \sinh L)$$

The 1-D Ising model

$$Z = (\cosh L)^N \sum_{s_1=\pm 1} \dots \sum_{s_N=\pm 1} \prod_{\langle ij \rangle} (1 + s_i s_j \tanh L)$$

- All terms with odd numbers of at least one spin variable do not contribute in the evaluation of the product in Z.
- 1-D ising model with open ends — no non-vanishing contributions from the products of spin variables, only contribution 2^N from the sum over all states.

$$Z = (2\cosh L)^N$$

- Periodic boundary conditions — one contribution $s_N s_1 \cdot s_1 s_2 \cdot \ldots \cdot s_{N-1} s_N (\tanh L)^N$:

$$Z = (2\cosh L)^N + (2\sinh L)^N$$

High temperature expansion

- With the abbreviation $u = tanhL$ we have

$$Z = (\cosh L)^s \sum_{s_1=\pm 1} \cdots \sum_{s_N=\pm 1} \prod_{\langle ij \rangle} (1 + s_i s_j u)$$

  with s the number of spin pairs dN.
- Only products which corresponds to closed paths contribute to Z

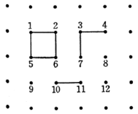


Fig. 4.12. An example of spin pairs whose contribution vanishes

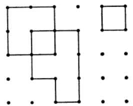


Fig. 4.13. An example of spin pairs whose contribution does not vanish

- With Ω_n denoting the numbers of figures with n bonds composed exclusively of polygons one gets expansions in powers of tanh $\frac{\beta J}{2}$

$$Z = 2^N (\cosh L)^s \left(1 + \sum_n \Omega_n u^n \right)$$

The low temperature expansion

- Number of spin pairs $s = Nd$. If there are r antiparalell spin pairs and $s - r$ parallel spin pairs then $\sum_{\langle ij \rangle} s_i s_j = (s - r) - r = s - 2r$.

$$Z = 2 \exp(sL) \left[1 + \sum_r \omega_r \exp(-2Lr) \right]$$

  with ω_r denoting the number of configurations with r antiparallel spins, and the coefficient 2 comes from the contribution by intverting all the spins.

- The lower T, the higher β and therefore also L. Thus for low T only small values of r contribute $\Rightarrow$ low temperature expansion

2-D systems — the dual lattice

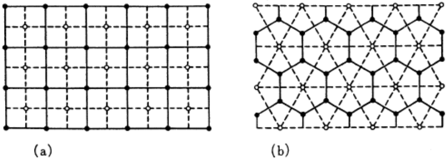


Fig. 4.14 **a, b.** Dual lattices. **(a)** A square lattice ↔ a square lattice; **(b)** a honeycomb lattice ↔ a triangular lattice

- Put ↑ spins at the dual lattice point inside the polygons in the figures of n bonds and put ↓ spins outside the polygons. This produces n antiparalle spin pairs in the dual lattice. Thus we get $\Omega_n = \omega_n^*$ and also $\omega_n = \Omega_n^*$.
- Obviously, we have $s^* = s$.

2-D systems — the dual lattice

- Partition function of the original lattice

$$Z(T) = 2^N (\cosh L)^s \left(1 + \sum_n \Omega_n (\tanh L)^n\right)$$

and of the dual lattice

$$Z^*(T) = 2\exp(sL)\left[1 + \sum_n \Omega_n \exp(-2Ln)\right]$$

- Because the square lattice is self-dual, we have

$$Z(T) = Z^*(T)\,.$$

Self-duality — the critical temperature

- Moreover, if we restrict ourselves to $J > 0 \quad (L > 0)$ we can define a temperature $T^*(T)$ with

$$\exp(-2L^*) = \tanh L \qquad T^* = \frac{J}{2kL^*}$$

- From this several symetric relations follow, e.g.

$$\exp(-2L) = \tanh L^*$$
$$\sinh 2L \sinh 2L^* = 1$$

- Moreover we have

$$Z^*(T*) = 2\exp(sL^*)2^{-N}(\cosh L)^{-s} Z(T)$$

- If there is only one singularity in $Z(T)$, there is also only one in $Z^*(T^*)$. Thus for $T = T_c$ $T = T^*$ and therefore

$$(\sinh 2L_c)^2 = 1 \qquad L_C \approx 0.4407$$

Transfer matrix method - 1-D Ising model

- Partition function

$$Z = \sum_{s_1=\pm 1} \dots \sum_{s_N=\pm 1} \prod K(s_1, s_2) \dots K(s_N, s_1)$$

  with

$$K(s_i, s_{i+1}) = \exp\left(C \frac{s_i + s_{i+1}}{2} + L s_i s_{i+1} \right)$$

$$C = \beta H \qquad L = \frac{\beta J}{2}$$

  and periodic boundary conditions $s_{N+1} = s_1$.
- Matrix formulation $Z = \mathrm{tr}\{K^N\} = \lambda_1^N + \lambda_2^N$

$$K = \begin{pmatrix} \exp(C+L) & \exp(-L) \\ \exp(-L) & \exp(-D+L) \end{pmatrix}$$

Transfer matrix method - 1-D Ising model

- Matrix formulation $Z = \mathrm{tr}\{K^N\} = \lambda_1^N + \lambda_2^N$

$$K = \begin{pmatrix} \exp(C+L) & \exp(-L) \\ \exp(-L) & \exp(-D+L) \end{pmatrix}$$

- Eigenvalues

$$\lambda_{1,2} = \exp L \cosh C \pm \sqrt{\exp(2L)\sinh^2 C + \exp(-2L)}$$

- For $H = 0$ and therfore $C = 0$

$$\lambda_1 = 2\cosh L \qquad \lambda_2 = 2\sinh L$$

- Magnetization

$$M = -\frac{\partial}{\partial H}(-kT \ln Z) = \frac{N \sinh C}{[\exp(-4L) + \sinh^2 C]^{1/2}}$$

- Susceptibility

$$\chi = -\frac{1}{\mu_0 \beta}\frac{\partial^2 \ln Z}{\partial H^2} = \frac{N}{kT}\exp\left(\frac{4J}{kT}\right)$$

Transfer matrix method - 2-D Ising model

- Again the system is considered with periodic boundary conditions $\Rightarrow$ 2-D lattice on a torus.
- The matrices $K(s_i, s_j)$ are replaced by $U(\boldsymbol{s}_i, \boldsymbol{s}_j)$ with $\boldsymbol{s}$ being the spin vector of the ith ring.
- Then again

$$Z = \mathrm{tr}\{U^N\} \qquad U(\boldsymbol{s}_i, \boldsymbol{s}_j) = \exp\left[-\Phi(\boldsymbol{s}_i, \boldsymbol{s}_j)\right]$$

- In the thermodynamic limit only the largest eigenvalue is important

$$\begin{aligned} Z &= \lambda_1^N + \lambda_2^N + \dots \\ &= \lambda_1^N \left[1 + \frac{\lambda_2}{\lambda_1}^N + \dots\right] \end{aligned}$$

- In order to have long-range order, the largest eigenvalue has to be degenerate, which is only possible in the thermodynamic limit.

Solution of the 2-D Ising model

- In a regular square lattice the partition function has the form

$$\frac{1}{N}\ln Z = \ln(2\cosh 2L) + \frac{1}{2\pi}\int_0^{\pi} \ln \frac{1}{2}(1+\sqrt{1-(4\kappa)^2\sin^2\phi})d\phi$$

  with $2\kappa = \frac{\tanh 2L}{\cosh 2L}$.
- Original paper: L.Onsager, Phys.Rev. **65**, 117(1944)
- For the solution via high-temperature expansion see e.g. Landau/Lifschitz Bd.5.

Scaling, Renormalization and Universality

- Start with some model $M(\boldsymbol{x}, \boldsymbol{p})$ defined on some scale ϵ with parameters $\boldsymbol{p}$.
- Now define new observable $\boldsymbol{x}'$ by coarse graining, e.g. integrating the old ones over a certain range. Then rescale the new variables, such that the model for the new variables is in the same space as the original one, but usually with different parameters $\boldsymbol{p}'$.
- Thus we get a map (or flow) $\boldsymbol{p} \mapsto \boldsymbol{p}'$ in the parameter space, with a semigroup property, the *renormalization group* (RG).
- If the system is self-similar it should be a fixed point of the transformation $\Rightarrow$ critical states are (unstable) fixed points of the RG transformation.
- Stable manifolds of these fixed points represent different models showing the same critical behaviour $\Rightarrow$ *universality*
- Critical exponents can be derived from the fixed point properties $\Rightarrow$ they are equal in one *universality class*

Characteristic function of a probability density

- Characteristic function

$$\hat{p}(k) = \int_{-\infty}^{\infty} dx \; \exp(ikx) \; p(x)$$

or inversely

$$p(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dk \; \exp(-ikx) \; \hat{p}(k)$$

- Moments of a probability density

$$m_n = \langle x^n \rangle = \int_{-\infty}^{\infty} dx \; x^n \; p(x)$$

- Then the moments are given by

$$m_n = (-i)^n \left. \frac{d^n}{dk^n} \hat{p}(k) \right|_{k=0} \qquad \hat{p}(k) = \sum_{n=0}^{\infty} \frac{m_n}{n!} (ik)^n$$

Cumulants

- The cumulants c_n of a pdf are defined as the derivatives of the logarithm of its characteristic function:

$$c_n = (-i)^n \, \frac{d^n}{dk^n} \ln \hat{p}(k) \bigg|_{k=0} \qquad \hat{p}(k) = \exp\left[\sum_{n=0}^{\infty} \frac{c_n}{n!} (ik)^n\right]$$

- The cumulants can be expressed by the moments:

$$\begin{aligned} c_1 &= \mu_1 && \text{mean} \\ c_2 &= \mu_2 && \text{variance} \\ c_3 &= \mu_3 && \propto \text{skewness} \\ c_4 &= \mu_4 - 3\mu_2^2 && \propto \text{excess kurtosis} \\ c_5 &= \mu_5 - 10\mu_2\mu_3 \end{aligned}$$

with the *central moments* μ_n

$$\mu_n = \langle x^n \rangle = \int_{-\infty}^{\infty} dx \, (x - m_1)^n \, p(x)$$

- Random variable X with $x = x_1 + x_2$. Then

$$
\begin{aligned}
p(x) &= \int_{-\infty}^{\infty} dx_1 p_1(x_1) \int_{-\infty}^{\infty} dx_2 p_2(x_2) \delta(x - x_1 - x_2) \\
p(x) &= \int_{-\infty}^{\infty} dx_1 p_1(x_1) p_2(x - x_2)
\end{aligned}
$$

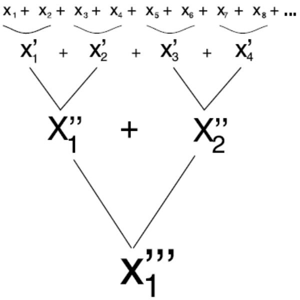
- Caracteristic function

$$\hat{p}(k) = \hat{p}_1(k)\hat{p}_2(k)$$

- Cumulants

$$c_n = c_n^{(1)} + c_n^{(2)}$$

Renormalization



1. Coarse graining:

$$\begin{aligned} \hat{p}^{(n+1)}(k) &= \left[\hat{p}^{(n)}(k)\right]^2 \\ c_l^{(n+1)} &= 2c_l^{(n)} \end{aligned}$$

2. Rescaling: $x_i^{(n)} = (x_j^{(n)} + x_{j+1}^{(n)})/2^\alpha$ leads to

$$c_k^{(n+1)} = 2^{1-k\alpha} c_k^{(n)}$$

3. Preserve variance:

$$\begin{aligned} c_2^{(n+1)} &= 2^{1-2\alpha} c_2^{(n)} \\ \Rightarrow \quad \alpha &= \frac{1}{2}\,. \end{aligned}$$

Central limit theorem

- Probability distribution characterized by its cumulants

$$p(c_1, \ldots, c_l, \ldots)$$

- Distribution $p^{(m)}$ of $X^{(m)}$ with $N = 2^m$ is then

$$p^{(m)} = p(2^{m(1-\alpha)}c_1, 2^{m(1-2\alpha)}c_1, 2^{m(1-3\alpha)}c_3, \ldots)$$

- and with $\alpha = 1/2$ and $N \to \infty$

$$p^{(\infty)} = p(c_1\sqrt{N}, c_2, c_3 = 0, \ldots, c_l = 0, \ldots)$$

  which is a Gaussian distribution.

- Gaussian distribution corresponds to the attractive fixed point of the renormalization process.

Stable Distributions

- Given two random variables X_1 and X_2 distributed according to the probability density p. p is called *stable*, if there are constant a, b and c such that $X = aX_1 + bX_2 + c$ is again distributed according to p.
- Examples for stable distributions are the *Gaussian* or Normal distribution

$$\rho(x) = \frac{1}{\sqrt{2\pi\sigma}} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right)$$

- the Cauchy-distribution

$$\rho(x) = \frac{1}{\pi} \frac{\gamma}{\gamma^2 + (x-\delta)^2}$$

- the Levy-distribution ($\delta < x < \infty$)

$$\rho(x) = \sqrt{\frac{\gamma}{2\pi}} \frac{1}{(x-\delta)^{3/2}} \exp(-\frac{\gamma}{2(x-\delta)})$$

- There are more stable distributions, but without closed form expressions.

Period doubling transition to chaos

- Starting point: unimodal map $f(x,a)$ on the unit interval $[0,1]$ depends on a parameter a. Fixed point $x^* = f(x^*, a)$. Stability $|f'(x^*(a), a)| < 1$. Fixed point becomes unstable for $|f'(x^*(a), a)| = 1$.
- The a period 2 orbit becomes stable, which is a fixed point of $f^2(x,a) = f(f(x,a))$. If there is a transformation that $T[f(x,a)] = f^2(x,a')$ in the vicinity of the fixed point, and more generally a transformation

  $$T[f^n(x,a)] = f^{n+1}(x,a')$$

  this induces a transformation $T_a : a_n \mapsto a_{n+1}$ for the values of a where the corresponding fixed points lose their stability.
- The fixed point of this transformation is the Feigenbaum point a_∞, the point of the transition to chaos.

Outlook

- (Renormalization group for the Ising Model)
- Self-organized criticality
- Power laws — mechanims and detection
- Computation at the edge of chaos