Introduction to Monte Carlo simulation methods: from Ising model to lattice gauge theory
Part 1: Ising model

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Organization of the lectures

- two main blocks: 1) Ising model, 2) SU(2) Yang-Mills theory
- lectures and exercises: theory and practical implementations

Lecture goals:

- critical phenomena in spin models
- Monte-Carlo simulations, algorithms
- gauge theory and gauge invariance
- simulations of non-perturbative phenomena (confinement)

Organization of the lectures

- lectures: 11.3. (14:00-15:30) 1) Ising and spin models,
  12.3. (10:00-11:30) 2) Monte-Carlo methods,
  13.3. (10:00-11:30) 3) gauge theories and lattice discretization,
  14.3. (10:00-11:30) Yang-Mills theory on the lattice,
  15.3. (9:00-10:30) 4) Towards lattice QCD
- exercises 1: 11.3.(15:30-16:30), introduction to first exercises: Ising model
- exercises 2: 12.3. (14:00-15:30), practical implementations, solutions
- exercises 3: 13.3. (14:00-15:30), exercises Yang-Mills theory
- exercises 4: 14.3. (14:00-15:30), practical implementations, solutions

https://www.tpi.uni-jena.de/~gbergner/compmethws2324.html

General motivation

Goal is quantum field theory on a space-time lattice:

- particle physics: relativistic quantum theory
- path integral formulation
- non-perturbative method: numerical lattice simulations

Approach starting from statistical mechanics:

- space-time lattice (Euclidean) $\leftrightarrow$ lattice of atoms in solid state physics
- Path $x(t) \leftrightarrow$ spin configuration
- $\exp(-S_E[x]/\hbar) \leftrightarrow \exp(-H(\{s\})/(k_B T))$
- continuum limit $\leftrightarrow$ critical phenomena (phase transitions)

Literature

Many different examples for Ising model simulations in various programming languages are avaiable online.

- Wipf, "Statistical Approach to Quantum Field Theory", Springer (2013)

The following books contain further information on simulations of pure gauge theory on the lattice:

- Gattringer, Lang, "Quantum Chromodynamics on the Lattice", Springer (2010)
- Montvay, Münster, "Quantum Fields on a Lattice", Cambridge University Press (1994)
- Smit, "Introduction to Quantum Field on a Lattice", Cambridge Lecture Notes in Physics (2002)
- Rothe, "Lattice Gauge Theories An Introduction" World Scientific (2005)

Goal of the first lecture: 1) Ising model

- introduction to physical applications
- thermodynamic quantities and observables
- basic analytic results for later comparison with data
- methods are in close connection to methods in lattice QFT

The Ising model

Simplified model for of a ferromanget:

- elementary magnets (spins $s_x \in \{-1, 1\}$) in Crystal-Lattice
- observations for $T < T_c$ (Curie-temperature): spontaneous magnetization
- first approximation: only nearest neighbor interactions

$$H(\{s_x\}) = -J \sum_{<x,y>} s_x s_y - h \sum_x s_x$$

$< x, y >$ pairs of next neighbors; h external magnetic field

- ferromagnetic: $J > 0$, antiferromagnetic $J < 0$
- expectation ($J > 0$): state with aligned spins favored, jump in preferred direction depending on the sign of h, thermal fluctuations might destroy alignment

The Ising model, some historical notes

- 1920: W. Lenz, E. Ising: Solution for 1D Ising model (no spontaneous magnetization)
- 1936: R. Peierls: Proof of spontaneous magnetization in 2D
- 1944: L. Onsager: analytic solution in 2D

D $>$ 2 no know analytical solution
Approximation methods:

- high and low temperature expansion
- mean field approximation
- numerical simulations ...

Ising model has become a standard model for statistical physics, which is used as a test and benchmark for new methods. (Even the most modern tools like conformal bootstrap or tensor networks.)

The canonical ensemble

- lattice Λ: $x = (x^1, \ldots, x^d)$, $x^\mu = n^\mu a$, $n^\mu = 1, \ldots, N^\mu$, $L^\mu = aN^\mu$, $V = \prod_{\mu=1}^{d} L^\mu$, (lattice spacing normalized to $a = 1$)
- spin at every lattice point: $s_x \in \mathcal{T}$, Ising model spin: $\mathcal{T} = \{-1, 1\}$
- Configuration $w = \{s_x | x \in \Lambda\}$, $w : \Lambda \to \mathcal{T}^V = \mathcal{T} \times \mathcal{T} \times \ldots$
- thermodynamic partition function ($\beta = 1/(k_B T)$)

$$Z_V(\beta, J, h) = \sum_{\{s_x\}} \exp(-\beta H(\{s_x\}))$$

- P probability of configuration $\{s_x\}$ in thermodynamic ensemble:

$$P(\{s_x\}, \beta, J, h) = \frac{1}{Z_V(\beta, J, h)} \exp(-\beta H(\{s_x\}))$$

Thermodynamic quantities

- thermodynamic average of observable O

$$\langle O \rangle_V(\beta, J, h) = \frac{1}{Z_V(\beta, J, h)} \sum_{\{s_x\}} O(\{s_x\}) \exp(-\beta H(\{s_x\}))$$

- e. g. (macroscopic) magnetization in volume V:

$$M_V = \frac{1}{V} \sum_x s_x; \quad \langle M \rangle_V = -\frac{\partial}{\partial h} f_V(\beta, J, h)$$

- free energy, free energy density

$$F_V(\beta, J, h) = -\frac{1}{\beta} \log Z_V(\beta, J, h); \quad f_V(\beta, J, h) = \frac{1}{V} F_V(\beta, J, h)$$

Thermodynamic quantities

- internal energy

$$U_V(\beta, J, h) = \langle H \rangle = -\frac{1}{Z_V}\frac{\partial}{\partial \beta}\sum_{\{s_x\}} \exp(-\beta H(\{s_x\})) = -\frac{\partial}{\partial \beta}\log Z_V(\beta, J, h)$$

- magnetic susceptibility

$$\chi_M = \frac{\partial}{\partial h}\langle M \rangle_V = \beta(\langle M^2 \rangle_V - \langle M \rangle_V^2)$$

- specific heat

$$C_V = \frac{1}{V}\frac{\partial}{\partial T} U_V = \langle H^2 \rangle - \langle H \rangle^2$$

Correlation functions, correlation length

- correlation function

$$G^{(n)}(x_1, \dots, x_n) = \langle s_{x_1} s_{x_2} \dots s_{x_n} \rangle$$

- two point correlation function

$$G^{(2)}(x_1 - x_2) = \langle s_{x_1} s_{x_2} \rangle \sim \exp(-|x_1 - x_2|/\xi)$$

  with correlation length ξ ($\langle M \rangle = 0$) determining long range behavior

- large distances: clustering

$$\langle s_{x_1} s_{x_2} \rangle \approx \langle s_{x_1} \rangle \langle s_{x_2} \rangle$$

- Hence at $\langle M \rangle \neq 0$:

$$\tilde{G}^{(2)}(x_1 - x_2) = \langle s_{x_1} s_{x_2} \rangle - \langle s_{x_1} \rangle \langle s_{x_2} \rangle \sim \exp(-|x_1 - x_2|/\xi)$$

Ising model in one dimension

Ising chain, periodic boundary conditions, $(K = \beta J)$

$$H(\{s_x\}) = -J \sum_{x=1}^{N} s_x s_{x+1} - h \sum_{x=1}^{N} s_x$$

$$\begin{aligned} Z_V(\beta) &= \sum_{s_1, s_2, \ldots, s_N} e^{K s_1 s_2 + \frac{1}{2}\beta h (s_1 + s_2)} e^{K s_2 s_3 + \frac{1}{2}\beta h (s_2 + s_3)} \ldots \\ &= \sum_{s_1, s_2, \ldots, s_N} T_{s_1 s_2} T_{s_2 s_3} \cdots T_{s_N s_1} = \mathrm{tr}\, T^N \end{aligned}$$

transfer matrix $(s = \{+1, -1\})$:

$$T = \begin{pmatrix} e^{K+\beta h} & e^{-K} \\ e^{-K} & e^{K-\beta h} \end{pmatrix}$$

Solution of the Ising model in one dimension

Diagonalization of transfer matrix

$$T = RDR^{-1}; \quad R = \begin{pmatrix} \cos\gamma & -\sin\gamma \\ \sin\gamma & \cos\gamma \end{pmatrix}; \quad D = \begin{pmatrix} \lambda_+ & 0 \\ 0 & \lambda_- \end{pmatrix}$$

$$\lambda_\pm = e^K \left(\cosh \beta h \pm \sqrt{\sinh^2 \beta h + e^{-4K}} \right)$$

$$\sin 2\gamma = \frac{e^{-2K}}{\sqrt{\sinh^2 \beta h + e^{-4K}}}; \quad \cos 2\gamma = \frac{\sinh \beta h}{\sqrt{\sinh^2 \beta h + e^{-4K}}}$$

partition function

$$Z_V(\beta) = \mathrm{tr}\, T^N = \lambda_+^N + \lambda_-^N = \lambda_+^N (1 + p^N); \quad p = \frac{\lambda_-}{\lambda_+} < 1$$

Ising chain thermodynamics

Diagonalization of transfer matrix:

$$f_V = -\frac{1}{\beta}\log\lambda_+ - \frac{1}{\beta N}\log(1+p^N) \rightarrow_{N\rightarrow\infty} f = -\frac{1}{\beta}\log\lambda_+$$

$$\langle M\rangle = \frac{1-p^N}{1+p^N}\cos 2\gamma \rightarrow_{N\rightarrow\infty} \frac{\sinh\beta h}{\sqrt{\sinh^2\beta h + e^{-4K}}}$$

spontaneous magnetization only in the limit of $T \rightarrow 0$

- U lowered by alignment of spins
- $s_x \rightarrow -s_x$ for part of the spins leads to $\Delta U = 4J$ at the boundary
- However: increase of entropy $\Delta S = k_B \log N$, since N possible positions of boundary

$\Rightarrow$ no lower $F = U - TS$ for aligned spins

Two dimensional Ising model

- 1936 shortly after Wilhelm Lenz and Ernst Ising found no phase transition in 1D: proof of $T_c > 0$ in 2D
- 1941 Kramers and Wannier T_c from duality transformations argument based on analysis of regions with aligned spins
- 1944 Lars Onsager: exact solutions form transfer matrix method

Phase diagram of the Ising model

external magnetic field:

- alignment of spins along magnetic field, disturbed by thermal fluctuations

$h \to 0$:

- low temperatures: ordered (aligned) spins, spontaneous magnetization ($M_{+/-}$ for $h \to 0_{+/-}$)
- high temperatures: thermal fluctuations dominant, disordered spins

There can be a phase transition between these two phases at a finite temperature (T_c).

Critical behavior

- relevant for critical behavior is the behavior of quantities in thermodynamic limit $f = \lim_{V\to\infty} f_V$

Phase transitions, order parameter ($\langle M\rangle$) shows non-analytic behavior

- first order: discontinuity of first derivative of partition function (order parameter)
- second order: second derivative of partition function shows discontinuous behavior (susceptibility or specific heat)

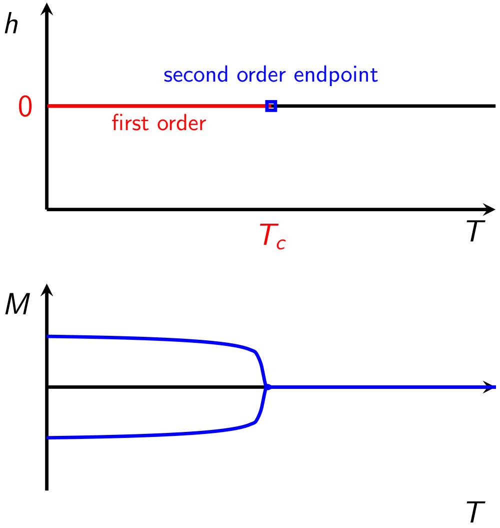
critical exponents characterize critical behavior

$$\langle M\rangle \sim \varepsilon^{\beta}; \qquad \varepsilon = \frac{|T - T_c|}{T_c}$$

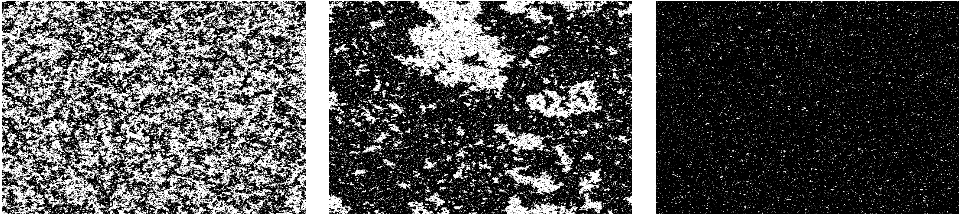
$$\chi_M \sim \varepsilon^{-\gamma}$$

$$C_V \sim \varepsilon^{-\alpha}, \qquad \xi \sim \varepsilon^{-\nu}$$

Phase diagram Ising model



Two dimensional Ising model in numerical simulations



- configurations at $K = 0.4$, $K \approx K_c$, $K = 0.5$ (700×700 Gitter)
- simulations show transition from ordered to disordered state
- $T \approx T_c$ scale invariance, domains on every scale

Solution by Onsager

longer calculations, solution for free energy

$$-\beta f = \log\cosh(2K) - 2K + \frac{2}{\pi}\int_0^{\frac{\pi}{2}} d\theta\ \log\left(1 + \sqrt{1 - \kappa^2 \sin^2\theta}\right)$$

$$\kappa = \frac{2\tanh(2K)}{\cosh(2K)}$$

$u(T)$, C_V depend on elliptic integrals; singularities of C_V indicate phase transition at $2K_c = \log(1 + \sqrt{2})$

Magnetization:

$T > T_c$: $\langle M \rangle = 0$

$T < T_c$: $\langle M \rangle = \left(1 - \sinh^{-4}(2K)\right)^{1/8}$

Approximation methods for the Ising model

Besides numerical simulations, a number of approximation methods have been established for the Ising model

- mean field approximation
- high temperature expansion
- low temperature expansion

General problem: Representation of non-analytic behavior at T_c in expansions

Low temperature expansion

Consider excitation of completely aligned state $E_0 = -dVJ - Vh$ taking into account the number of such configurations. Spins in region X flipped: number of spins determined by volume $n = |X|$, boundary of volume (pairs of misaligned spins) $p = |\partial X|$

$$Z_V = e^{-\beta E_0} \sum_{n,p} z^n u^p G_V(n,p), \quad z = e^{-2\beta h}, \quad u = e^{-2\beta J},$$

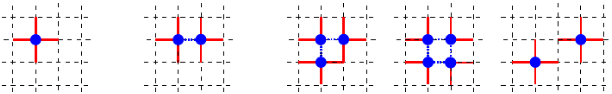
G_V number of configurations with n and p.
alternatively ($h = 0$): $H = E_0 + 2J \sum_{<x,y>} (1 - \delta(s_x, s_y))$

$$Z_V = e^{-\beta E_0} \sum_{s_x} e^{-2\beta J n_f[\{s_x\}]}$$

n_f number of bonds with different sign on both sides

Low temperature expansion

$$Z_V = e^{-\beta E_0}(1 + Vzu^4 + 2Vz^2u^6 + V(z^4 + 6z^3 + (V-5)z^2/2)u^8 + \dots)$$



Derivative of f is magnetization

$$\langle M \rangle = 1 - 2zu^4 - 8z^2u^6 - (8z^4 + 36z^3 - 10z^2)u^8 + \dots$$

critical temperature can be determined from convergence radius of expansion

$$\langle M \rangle = \sum a_l u^{2l} \sim \left(1 - \frac{u^2}{u_c^2}\right)^{\beta}$$

Low temperature expansion

Convergence radius $R = \lim_{l \to \infty} \frac{a_l}{a_{l-1}}$, determined by fit of

$$\frac{a_l}{a_{l-1}} = \frac{1}{u_c^2} - \frac{1+\beta}{u_c^2}\frac{1}{l}$$

To determine u_c (T_c) and β (critical exponent).

Low temperature expansion:

- Ansatz: expansion around configuration that minimizes H
- Similar to semiclassical expansion or weak coupling expansion in QFT

High temperature expansion

High temperatures, expansion for $\beta \ll 1$
naive expansion ($h = 0$):

$$Z_V = \sum_{\{s_x\}} \prod_{<x,y>} e^{K s_x s_y} = \sum_{\{s_x\}} \prod_{<x,y>} \left(1 + K s_x s_y + \frac{(K s_x s_y)^2}{2!} + \ldots\right)$$

Summation over all spin configurations: contributions with odd number of spins at a lattice point vanish.

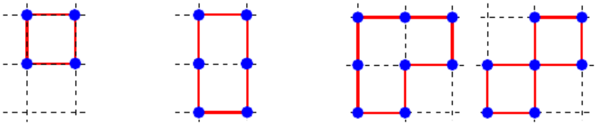
$$Z_V = 2^V \left(1 + K^2 \frac{2V}{2} + \ldots\right)$$

High temperature expansion

More efficient expansion (character expansion):
$e^{Ks_x s_y} = \cosh(K)(1 + vs_x s_y), \ v = \tanh(K)$

$$Z_V = (\cosh K)^{2V} \sum_{\{s_x\}} \prod_{<x,y>} (1 + vs_x s_y)$$

$$Z_V = (\cosh K)^{2V} 2^V \left(1 + Vv^4 + 2Vv^6 + \dots\right)$$



High temperature expansion

Expansion of susceptibility can be derived from the expansion of two point function ($\langle M \rangle = 0$)

$$\chi = \frac{1}{V} \sum_{x,y} \langle s_x s_y \rangle$$

Graphs with insertions s_x and s_y.

$$\chi = 1 + 4v + 12v^2 + 36v^3 + 100v^4 + 276v^5 + 740v^6 + \dots$$

High temperature expansion comparable to expansion in lattice QFT

- „strong coupling" expansion
- hopping parameter expansion

Mean field approximation

Main idea of this approach:

- interaction of neighboring spins replaced by interaction with mean field
- self consistency equation for mean field
- factorization of Boltzmann measure
- mean field approximation predicts phase transition
- precision depends on coordination number: the larger the number of interacting spins the better the precision

$$T_{c,mf} = 2dJ$$

Summary

Ising model

- playground for investigations of numerical methods and approximations
- lattice QFT: closely related to physics of statistical models
- 2D Ising model: Exact solutions allow benchmark of numerical methods
- 3D and higher: only numerical solutions and approximation methods