The Ising-Model

Model of interacting quantum spins in a magnetic field, introduced as model for ferromagnetism by Wilhelm Lenz (~ Runge-Lenz vector) and Ernst Ising in Ising's PhD thesis (Hamburg, 1924).
(10.5.1900 - 11.5.1998)

[Ising later became teacher, emigrated via Luxemburg to the USA. After Onsager's solution (1944) he became professor at Bradley university, Peoria, Illinois, but never published another journal article.]

Hamiltonian of general Ising model (N lattice sites): *

$$\mathcal{H} = -\frac{1}{2}\sum_{i,j=1}^{N} J_{ij}\, \sigma_i \sigma_j - \mu_B B \sum_{i=1}^{N} \sigma_i \qquad \sigma_i \in \{+1,-1\}$$

specifically for translation-invariant, isotropic nearest-neighbor interaction:

$$\boxed{\mathcal{H} = -J \sum_{\langle i,j\rangle} \sigma_i \sigma_j - \mu_B B \sum_i \sigma_i}$$

sum over NN pairs, each pair counted <u>once</u>

- important special case: $B = 0$
- trivial single-spin (noninteracting) limit: $J = 0$

- ferromagnetic/antiferromagnetic coupling for $J \gtrless 0$
- properties strongly dependent on lattice (i.e. also on dimensionality)

* more general spin Hamiltonian:

$$\mathcal{H} = -\frac{1}{2} \sum_{ij} \vec{S}_i \cdot \overleftrightarrow{I}_{ij} \cdot \vec{S}_j$$

↑ Eigenvalues $\pm\frac{1}{2}\hbar$

(isotropic) Heisenberg model: $\overleftrightarrow{I}_{ij} = I_{ij}\,\mathbb{1}$

Ising model: $(I_{ij})_{\mu\nu} = I_{ij}\,\delta_{\mu 3}\,\delta_{\nu 3}$

use scaled interactions $J_{ij} = (\frac{1}{2}\hbar)^2 I_{ij}$

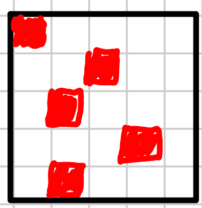
possible visualization: $\underbrace{\uparrow\ \uparrow}_{J}\ \downarrow\ \uparrow\ \downarrow\ \downarrow\ \uparrow \qquad \uparrow \vec{B}$

spins: up or down

$$\sigma_i = \frac{2}{\hbar} S_i^z \quad (\vec{S}_i : \text{spin vector})$$

alternative visualizations:

+ − − + +
− + − + −
− + + − +
+ − − + −
+ + − + +



closely related: lattice gas model (lattice sites occupied/empty):

$$\mathcal{H}_{LGM} = U_{NN} \sum_{\langle ij \rangle} n_i n_j - \mu \sum_i n_i \ ; \quad n_i \in \{0, 1\}$$

↑ chem. potential (in grand canonical ensemble)

Excursion: reminder on statistics (cf. Landau/Binder chapter 2)

partition function in canonical ensemble:

$$Z = \sum_{\substack{\text{all}\\\text{states}}} e^{-\mathcal{H}/k_B T} = \sum_{\text{states}} e^{-\beta \mathcal{H}}$$

free energy $F = -k_B T \ln Z$

internal energy
$$E = \frac{\sum \mathcal{H} e^{-\beta\mathcal{H}}}{\sum e^{-\beta\mathcal{H}}}$$
$$= \frac{-\partial Z/\partial\beta}{Z} = -\frac{\partial \ln Z}{\partial\beta} = \frac{\partial(\beta F)}{\partial\beta}$$
$$= -T^2 \frac{\partial(F/T)}{\partial T} = F - T\frac{\partial F}{\partial T}$$

entropy $S = -\frac{\partial F}{\partial T}$ (e.g. from $F = E - TS$)

Specific heat: $C = \frac{\partial E}{\partial T} = \frac{\partial E}{\partial\beta}\frac{\partial\beta}{\partial T}$

$$\overset{*}{=} \frac{\langle \mathcal{H}^2\rangle - \langle\mathcal{H}\rangle^2}{k_B T^2}$$

Very useful in simulations: avoids numerical differentiation.

magnetic dipole moment $m = \langle \mu_B \sum_i \sigma_i \rangle$
$= \frac{1}{\beta Z}\frac{\partial Z}{\partial B} = \frac{1}{\beta}\frac{\partial \ln Z}{\partial B}$; $M = \frac{m}{N\mu_B}$ } for Ising model

phase transitions: singularities in thermodynamic quantities (i.e. points/lines/planes in phase space where F, E, m etc. are nonanalytic).

However: F is always continuous (as function of T, B)

Classification according to Ehrenfest:

1st order transition: discontinuities in first derivatives of F

2nd order transition:
- continuous first derivatives of F
- discontinuities in second derivatives of F

Examples: liquid-gas transition etc.

Note: systems with a finite number of states cannot undergo phase transitions since a finite sum of analytic functions is analytic:

$$Z = \sum_{s=\text{state}1}^{\text{state } s_{max}} e^{-\beta \mathcal{H}_s} \quad \text{analytic}$$

Critical exponents: characterize behavior near 2nd order transitions

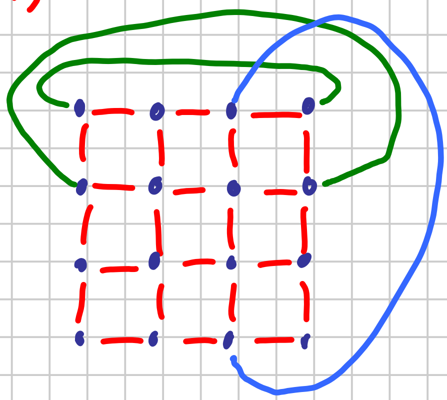
$$\left.\begin{array}{lll} \text{magnetization} & m = m_0\, \varepsilon^{\beta} \\ \text{susceptibility} & \chi = \chi_0\, \varepsilon^{-\gamma} \\ \text{specific heat} & C = C_0\, \varepsilon^{-\alpha} \\ \text{correlation length} & \xi = \xi_0\, \varepsilon^{-\nu} \end{array}\right\} \varepsilon = \left|1 - \frac{T}{T_c}\right|$$

magnetization at T_c: $m \propto B^{1/\delta}$

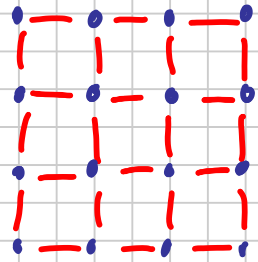
Ising model: simulation

1^{st} consideration: Hamiltonian for finite-size system, i.e. boundary conditions

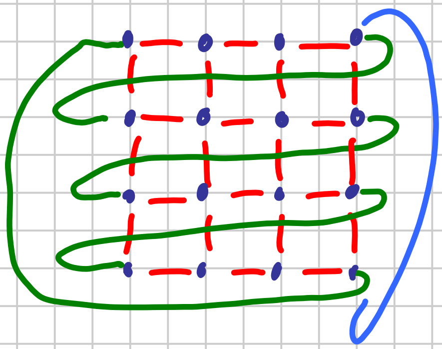
(i) conventional choice: periodic boundary conditions
$\Rightarrow$ all sites equivalent



(ii) other extreme: open/free edge boundary conditions
$\Rightarrow$ inner + surface sites

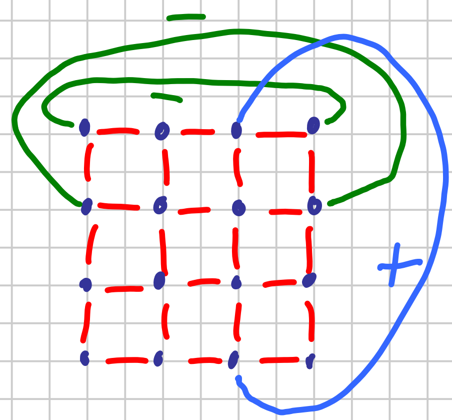


(iii) screw periodic boundary cond.
easy to implement on 1d vector $\Rightarrow$ introduces seam

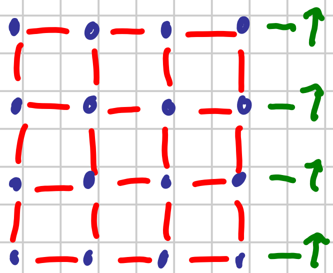


(iv) antiperiodic boundary conditions:

flip sign of interaction along some boundaries
$\Rightarrow$ generate odd number of domain walls (e.g. 1) at $T \to 0$



(v) fixed or mean-field boundary conditions: boundary sites couple to external medium



Possibilities can be combined/mixed ...

Metropolis importance sampling Monte Carlo scheme

(i) choose initial spin configuration

(ii) select site i

(iii) calculate $\Delta E = E\{\sigma_\ell; \sigma_i \to -\sigma_i\} - E\{\sigma_\ell\}$

(iv) Metropolis step:

- if $\Delta E < 0$: accept move
- else generate random number $r \in [0,1)$
  - if $r < \exp[-\Delta E / k_B T]$: flip spin ($\sigma_i \to -\sigma_i$)
  - else: keep state

(v) after warm-up: measure

$$\left.\begin{aligned} &nsum \mathrel{+}= 1 \\ &msum \mathrel{+}= mag\{\sigma_\ell\} \\ &Esum \mathrel{+}= E\{\sigma_\ell\} \\ &\vdots \end{aligned}\right\} \text{compute internally or print for external analysis}$$

(vi) enough sweeps ($N = L^d$ attempted spin flips)?

- yes: compute averages + error bars (if done internally)
- no:

<u>note:</u> ΔE depends only on nearest neighbors of site i, specifically only on number of up spins in neighborhood (and σ_i)
$\rightsquigarrow$ look-up table possible

Home work (see course page)

- 2007/11/22 Monte Carlo simulation of 2D Ising model (due: 2007/11/29)
  - Write a Monte Carlo program for computing energy and magnetization of the 2 D square Ising model using single-spin flips (possibly using the template C program linked below).
  - Compute E(T), |M(T)| in a useful temperature range for lattices with linear sizes between about 4 and 20-40
  - Plot Binder's 4th order cumulant $U_4(T)=1-\langle M^4\rangle/(3\langle M^2\rangle^2)$ and determine T_c
  - Optional: determine specific heat and susceptibility at selected temperatures

Example:

Magnetization (10^5 sweeps)