Computer Simulations in Statistical Physics

lecture 8+9
2006/11/16+21

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Contents

- Ising model
  - Hamiltonian
  - Ernst Ising & Wilhelm Lenz
  - properties in 1 dimension
  - [2D: duality transformation (Kramers, Wannier) + Onsager]
  - observables: E, M + statistics (Z, F)
  - mean-field solution ($D=\infty$)
  - finite size versions

    open / closed / fixed / mixed bc's

$\sim$ (grand canonical) lattice gas model w NN interaction

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: $H=0$
- 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 $\pm\frac{1}{2}\hbar$

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

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 $F = E - TS$)

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:

1^{st} order transition: discontinuities in first derivatives of F

2^{nd} 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:

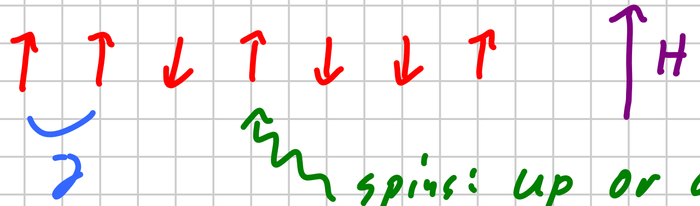
$$Z = \sum_{s=\text{state}1}^{\text{state } s_{max}} e^{-\beta \mathcal{H}_s} \quad \text{analytic}$$

Critical exponents: characterize behavior near 2^{nd} order transitions

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

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

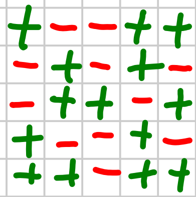
possible visualization:

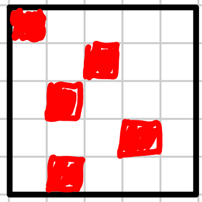


spins: up or down

$$\sigma_i \equiv s_i^z \qquad (\vec{s}_i: \text{spin vector})$$

alternative visualizations:





closely related: lattice gas model:

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

μ: chem. potential (in grand canonical ensemble)

Mean-field solution of the Ising model

Mean-field approximation: correlations of the form

$$\langle (\sigma_i - \langle \sigma_i \rangle)(\sigma_j - \langle \sigma_j \rangle) \rangle$$

are neglected.

(remember conditional probabil.: if a given spin is known to be up, surrounding spins are more likely to be up/down in ferro/antiferromagnetic model)

For homogeneous case $(\langle \sigma_i \rangle = \langle \sigma_j \rangle \equiv \langle \sigma \rangle = M)$

$$0 \stackrel{!}{=} (\sigma_i - \langle \sigma \rangle)(\sigma_j - \langle \sigma \rangle)$$

$$= \sigma_i \sigma_j - (\sigma_i + \sigma_j) \langle \sigma \rangle + \langle \sigma \rangle^2$$

$$\Rightarrow \quad \sigma_i \sigma_j \rightarrow (\sigma_i + \sigma_j) \langle \sigma \rangle - \langle \sigma \rangle^2$$

$$\mathcal{H} = -J \sum_{\langle ij \rangle} \sigma_i \sigma_j - H \sum_i \sigma_i$$

$$\approx \mathcal{H}_{MF} = -J \sum_i \sigma_i \sum_{\substack{j \\ j\,\text{NN of } i}} \langle \sigma \rangle - H \sum_i \sigma_i$$

$$= -(\underbrace{H + zJ\langle \sigma \rangle}_{H_{eff}}) \sum_i \sigma_i$$

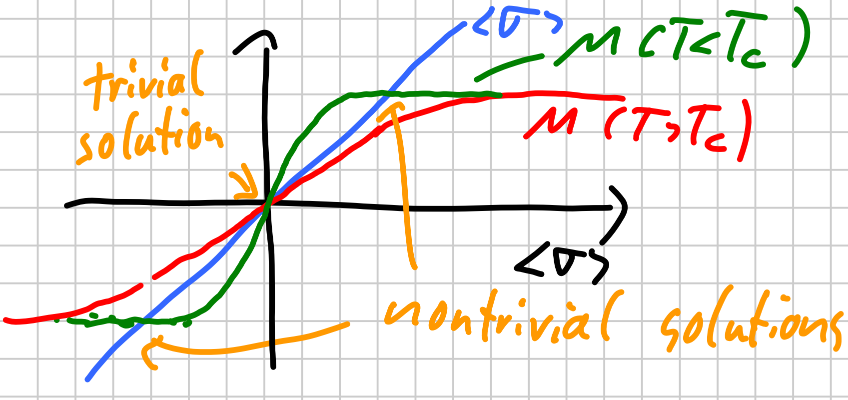
z: coordination number (# of nearest neighbors)

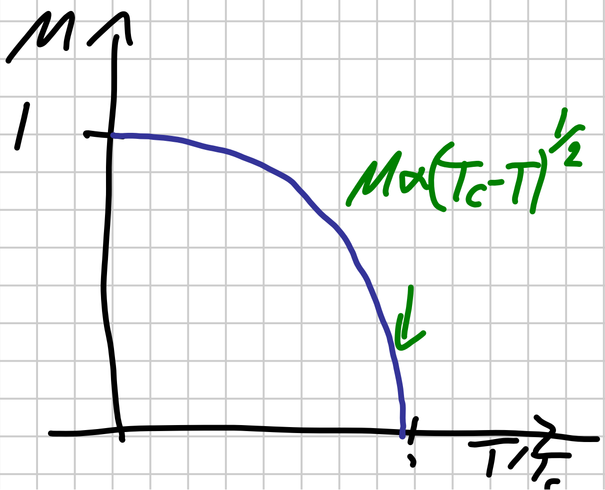
effective single-spin Hamiltonian with self-consistency condition

$\Rightarrow$ partition function $$\mathcal{Z} = \left(\sum_{\sigma_i = \pm 1} \exp\left(\sigma_i \frac{H + zJ\langle\sigma\rangle}{k_B T}\right)\right)^N$$
$$= \left(2\cosh \frac{H + zJ\langle\sigma\rangle}{k_B T}\right)^N$$

$\Rightarrow$ magnetization $$M = \langle \sigma \rangle = \frac{1}{N} k_B T \frac{\partial \ln \mathcal{Z}}{\partial H}$$
$$= k_B T \frac{\partial}{\partial H} \ln\left(\cosh \frac{H + zJ\langle\sigma\rangle}{k_B T}\right)$$
$$= \tanh \frac{H + zJ\langle\sigma\rangle}{k_B T}$$

graphical solution:





$$\tanh(x) = \frac{e^{x} - e^{-x}}{e^{x} + e^{-x}} \qquad e^{x} = \sum_{n=0}^{\infty} \frac{1}{n!} x^{n}$$

$$= \frac{2(x + \frac{1}{6}x^{3} + \dots)}{2(1 + \frac{1}{2}x^{2} + \dots)} = \left(x + \frac{1}{6}x^{3}\right)\left(1 - \frac{1}{2}x^{2}\right) + \mathcal{O}(x^{5})$$

$$= x - \frac{1}{3}x^{3} + \mathcal{O}(x^{5})$$

$$m = \tanh \beta J^{*} m$$

$$\cancel{m} \approx \beta J^{*} \cancel{m} \left[1 - \frac{1}{3}(\beta J^{*} m)^{2}\right]$$

$$\frac{1}{\beta J^{*}} = 1 - \frac{1}{3}(\beta J^{*})^{2} m^{2} \qquad \beta_c J^{*} = 1$$

$$m^{2} = \frac{1 - \frac{1}{\beta J^{*}}}{\frac{1}{3}(\beta J^{*})^{2}} \qquad k_B T_c = J^{*}$$

$$= 3\left(1 - \frac{T}{T_c}\right)$$

$$m = \sqrt{3} \sqrt{1 - \frac{T}{T_c}}$$

$$\tanh' = \left(\frac{\sinh}{\cosh}\right)' = 1 - (\tanh)^{2} \xrightarrow{x \to 0} 1$$

$$\tanh'' = -2 \tanh \tanh' = -2 \tanh (1 - \tanh^{2})$$

$$= -2 \tanh + 2 \tanh^{3}$$

$$\tanh''' = -2(1 - \tanh^{2})(1 - 3\tanh^{2}) \xrightarrow[x \to 0]{} -2$$