Computer Simulations in Statistical Physics

lecture 10
2006/11/23

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+ solution in 1D
+ approaches for 2D square lattice
+ boundary conditions
+ Monte-Carlo algorithm

Ising model: solution in 1 dimension

(i) simple case: open chain, no magnetic field

$$\mathcal{H} = -J\sum_{i=1}^{N-1} \sigma_i \sigma_{i+1} = -J \sum_{i=2}^{N} \sigma_{i-1}\sigma_i$$

$$Z = \sum_{\sigma_1=\pm} \sum_{\sigma_2=\pm} \cdots \sum_{\sigma_N=\pm} e^{-\beta \mathcal{H}\{\sigma_\ell\}}$$

Trick: introduce new variables $\{s_i\}$ with

$$s_1 = \sigma_1 \, ; \quad s_i = \sigma_i \sigma_{i-1} \text{ for } i \geq 2 \quad \left(\Rightarrow \ \sigma_i = \prod_{j=1}^{i} s_j\right)$$

$$\Rightarrow \ \mathcal{H} = -J \sum_{i=2}^{N} s_i$$

$$Z = \left(\sum_{s_1=\pm}\right)\left(\sum_{s_2=\pm} e^{-\beta J s_2}\right)\left(\sum_{s_3=\pm} e^{-\beta J s_3}\right)\cdots\left(\sum_{s_N=\pm 1} e^{-\beta J s_N}\right)$$

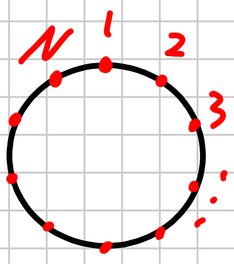
$$= 2\,\left(2\cosh(\beta J)\right)^{N-1} = 2^N\left[\cosh(\beta J)\right]^{N-1}$$

$$\Rightarrow \ E(\beta) = -\frac{\partial \ln Z}{\partial \beta} = -(N-1)\tanh(\beta J)$$

$$E(T) = -(N-1)\, J \tanh(J/k_B T)$$

∞ often differentiable for all $0 < T < \infty$ $\rightsquigarrow$ no finite-T phase trans.

(ii) more relevant case: periodic boundary conditions (+ magnetic field)



$$\mathcal{H} = -J \sum_{i=1}^{N} \sigma_i \sigma_{i+1} - \mu_B B \sum_{i=1}^{N} \sigma_i \qquad (\sigma_{N+1} = \sigma_1)$$

rewrite as sum over bonds only (not sites):

$$\mathcal{H} = \sum_{i=1}^{N} [\underbrace{-J\sigma_i\sigma_{i+1} - \tfrac{1}{2}\mu_B B(\sigma_i + \sigma_{i+1})}_{E_{bond}(\sigma_i,\sigma_{i+1})}]$$

$$= \sum_{i=1}^{N} E_{bond}(\sigma_i, \sigma_{i+1})$$

task: compute $\quad Z = \sum_{\{\sigma_i\}} \prod_{i=1}^{N} \underbrace{e^{-\beta E_{bond}(\sigma_i,\sigma_{i+1})}}_{P(\sigma,\sigma')}$

idea: rewrite as product of transfer matrices

$$\begin{array}{cccc} & \sigma=+1 & \sigma=-1 & \\ P = & \begin{pmatrix} e^{\beta(J+\mu_B B)} & e^{-\beta J} \\ e^{-\beta J} & e^{\beta(J-\mu_B B)} \end{pmatrix} & & \begin{array}{l}\sigma'=+1\\ \sigma'=-1\end{array} \end{array}$$

$Z = \mathrm{Tr}(P^N)$

trace of matrix A: $tr(A) = \sum_{i=1}^{N} A_{ii}$

trace is invariant under unitary transformations

$\rightsquigarrow$ trace of A is sum of eigen values of A

" " A^N " " " (eigen values)^N " "

$$\boxed{\begin{aligned} &\Rightarrow \quad Z = (p^+)^N + (p^-)^N \quad \text{where} \\ &p_\pm = e^{\beta J}\cosh(\beta\mu_B B) \pm \sqrt{e^{2\beta J}\sinh^2(\beta\mu_B B) + e^{-2\beta J}} \end{aligned}}$$

(special case $B=0$: $p_\pm = e^{\beta J} \pm e^{-\beta J}$ — bc's important at $T\to 0$

$\Rightarrow \quad Z = [2\cosh(\beta J)]^N + [2\sinh(\beta J)]^N$)

survives in thermod. limit

magnetization (in thermodynamic limit):

$$m = \frac{1}{\beta}\frac{\partial \ln Z}{\partial B} = \frac{1}{\beta} N \frac{\partial \ln \rho^+}{\partial B} = \frac{N}{\beta}\frac{\partial \ln(\rho^+/e^{\beta J})}{\partial B}$$

$$= N\mu_B \frac{\sinh(\beta\mu_B B)}{\sqrt{\sinh^2(\beta\mu_B B)+e^{-4\beta J}}}$$

no finite-temperature magnetism: $m \xrightarrow{B\to 0} 0$ for $T>0$

(but ground state fully polarized: $m = \pm N\mu_B$ for $T=0$)

Explanation: lowest energy excitations are domain walls (cost $2J$) which disconnect the system.

On the basis of these results, Ising and Lenz discarded the model as irrelevant for (finite T) magnetism.

Ising model on the 2d square lattice

Sketch of Kramers' and Wannier's determination of T_c using a duality transformation.

(i) use bond-product representation of partition function:

$$Z = \sum_{\{\sigma\}}\prod_{\langle ij\rangle} e^{\beta J \sigma_i \sigma_j}$$

$$(\sigma_i\sigma_j)^2 = 1 \Rightarrow e^{\beta J\sigma_i\sigma_j} = \cosh(\beta J) + \sigma_i\sigma_j \sinh(\beta J)$$

$$= \cosh(\beta J)[1+\sigma_i\sigma_j \tanh(\beta J)]$$

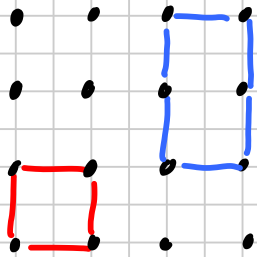
high-temperature expansion

$\rightsquigarrow Z = 2^N[\cosh(\beta J)]^{qN/2}\sum_{\nu=0}^{\infty} n(\nu)[\tanh(\beta J)]^{\nu}$ where

$n(\nu)$ = number of closed graphs of length ν; $n(0)=1$

valid for arbitrary dimension

examples:

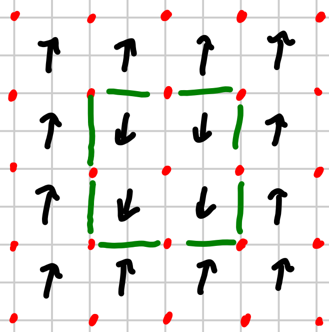


(application to $d=1$ with periodic bc's: $n(\nu) = \begin{cases} 1 & \text{for } \nu = 0 \\ 1 & \text{''} \ \nu = N \\ 0 & \text{else} \end{cases}$;

$q=2 \Rightarrow Z = 2^N [\cosh(\beta J)]^N [1 + [\tanh(\beta J)]^N]$)

(ii) for low-temperature expansion, classify clusters of flipped (down) spins in environment of majority (up) spins by their domain walls

domain walls in 2d: closed graphs on dual lattice

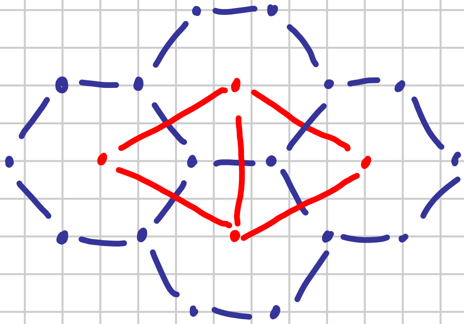


energy cost: $2J \cdot$ length of domain wall

$$\Rightarrow Z = e^{qN\beta J} \sum_{\nu=0}^{\infty} m(\nu)\, e^{-2\beta J \nu} \quad \text{(only } D=2\text{)}$$

$m(\nu)$: # closed graphs of length ν on dual lattice

2d square lattice is self-dual $\Rightarrow n(\nu) = m(\nu)$

(

another dual pair:

honeycomb lattice $\leftrightarrow$ triangular lattice)

define $j = \beta J$; $e^{-2j} = \tanh(j^*)$; $T^* = J/k_B j^*$

use • high-T expansion for j^*, T^* and low-T expansion for T, j

• only single singularity: $T_c = T_c^*$

$$\rightsquigarrow \quad \sinh(2 j_c) = 1$$

$$\Rightarrow \quad \frac{J}{k_B T_c} = \frac{1}{2} \operatorname{arsinh}(1) = \frac{1}{2} \ln(\sqrt{2}+1) \approx 0.4407$$

$$\boxed{T_c \approx 2.2692 \, \frac{J}{k_B}}$$

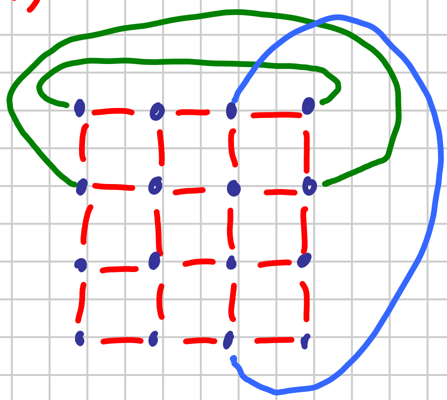
Critical exponents: $\alpha = 0$, $\beta = \frac{1}{8}$, $\gamma = \frac{7}{4}$, $\delta = 15$

[For more details, see: thermodynamics script by Prof. P. van Dongen]

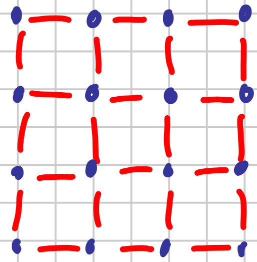
Ising model: simulation

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

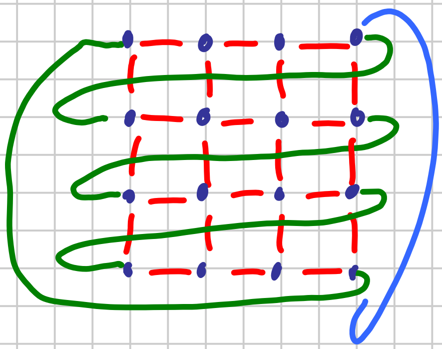
(i) conventional choice: periodic boundary conditions
$\Rightarrow$ all sites equivalent



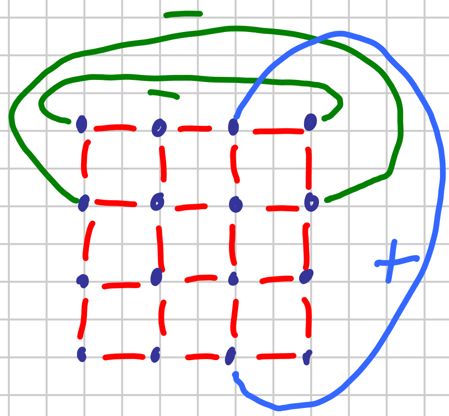
(ii) other extreme: open/free edge boundary conditions
$\Rightarrow$ inner + surface sites



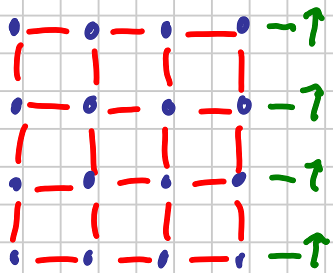
(iii) screw periodic boundary cond.
easy to implement on 1d vector $\Rightarrow$ introduces seam



(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

$$\left.\begin{aligned} nsum &\mathrel{+}= 1 \\ msum &\mathrel{+}= mag\{\sigma_\ell\} \\ Esum &\mathrel{+}= E\{\sigma_\ell\} \\ &\vdots \end{aligned}\right\}$$

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