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:

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

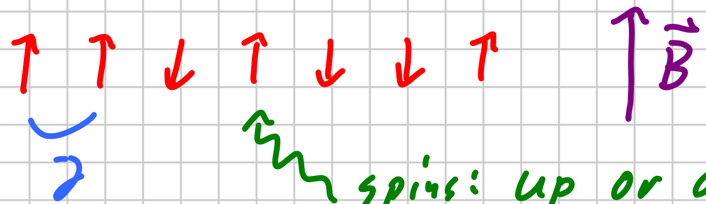
Eigenvalues $\pm\frac{1}{2}\hbar$

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

possible visualization:



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

alternative visualizations:

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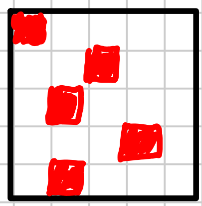


closely related: lattice gas model (lattice sites occupied/empty):

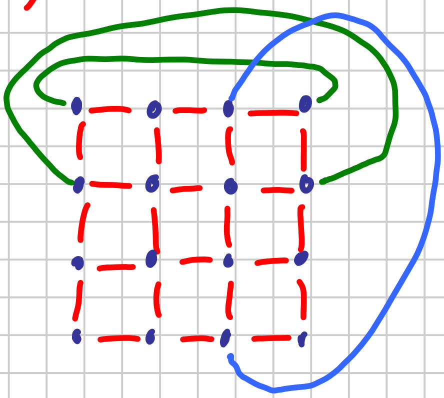
$$\mathcal{H}_{LGM} = U_{NN} \sum_{\langle ij \rangle} n_i n_j - \mu \sum_i n_i \; ; \quad n_i \in \{0, 1\}$$

chem. potential (in grand canonical ensemble)

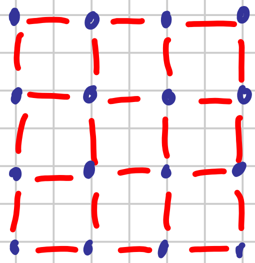
Ising model: simulation

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

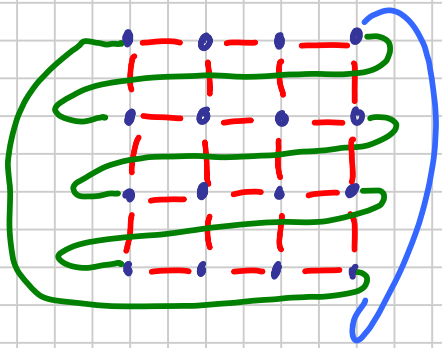
(i) conventional choice: periodic boundary conditions
$\Rightarrow$ all sites equivalent



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

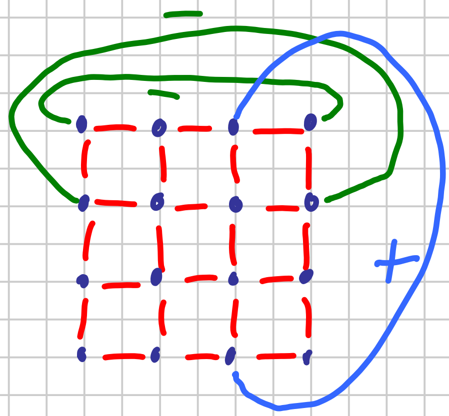


(iii) screw periodic boundary cond.
easy to implement on 1d vector $\Rightarrow$ introduces seam

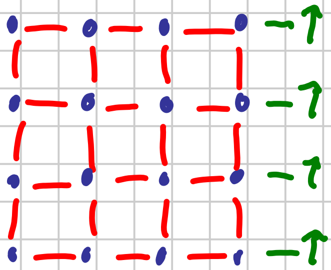


(iv) antiperiodic boundary conditions:

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: → back to (ii)

<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)