The one- and two-dimensional Ising model

Master seminar on statistical physics

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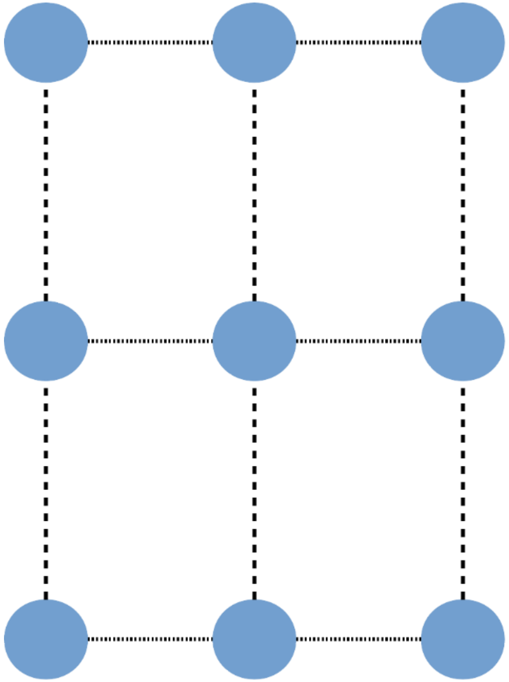
Overview

- Basic idea and motivation
- History
- 1D-Ising model:
    - Ising’s original approach
    - Transfer matrix method
- 2D-Ising model:
    - Transfer matrix method
    - Onsager’s exact solution
- Metropolis Algorithm (Monte Carlo simulation)
- Achievements of the Ising model

Basic Idea [1], [2], [4], [5]

Ferromagnet:

- Lattice
- Atom on each site → magnetic moment



Basic Idea

Ferromagnet:

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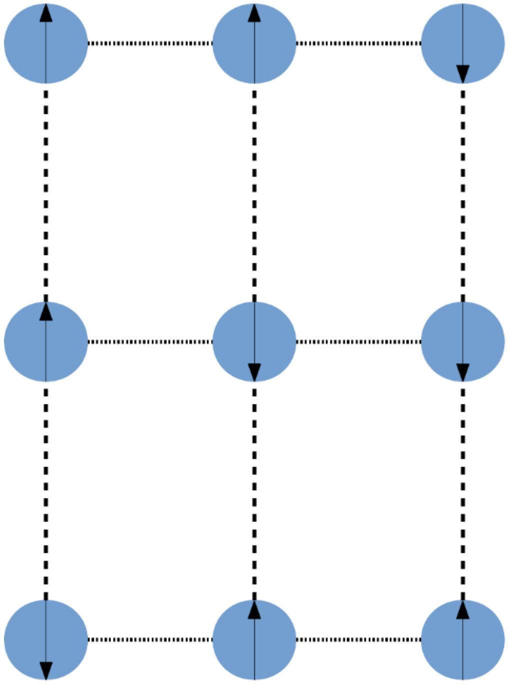


Basic Idea

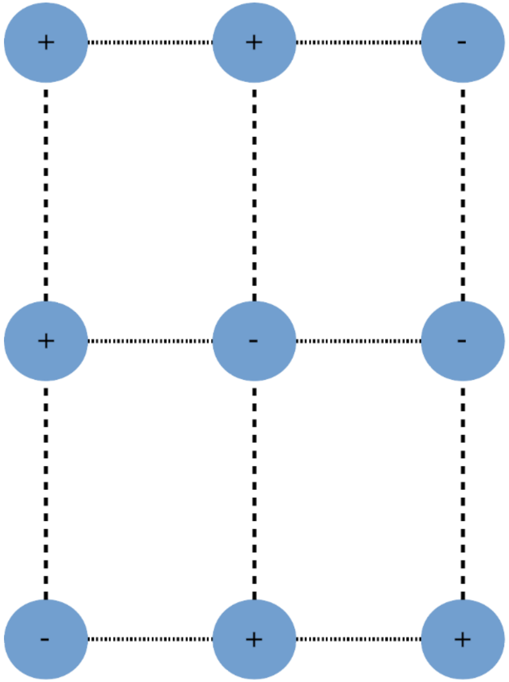
Ferromagnet:

- Lattice
- Atom on each site → magnetic moment
- Discrete variable $\sigma_{\mathrm{i}} = \pm 1$

  → 2^N configurations for N sites
- Nearest neighbour interaction

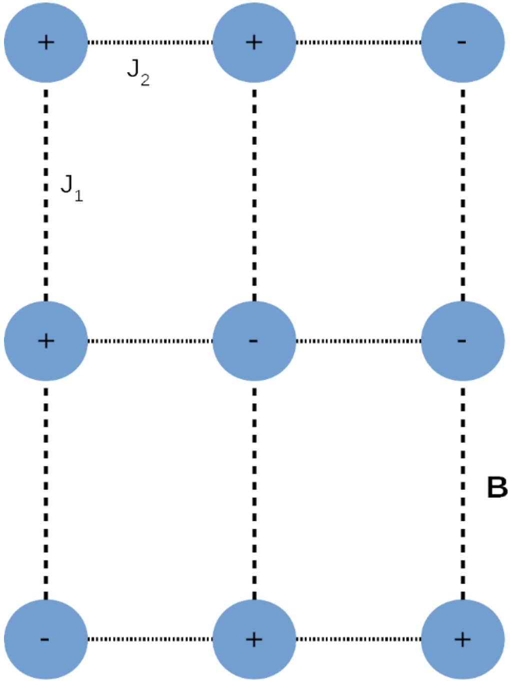
  → tends to make next spins same

  → spontaneous magnetization (PT)



Basic Idea

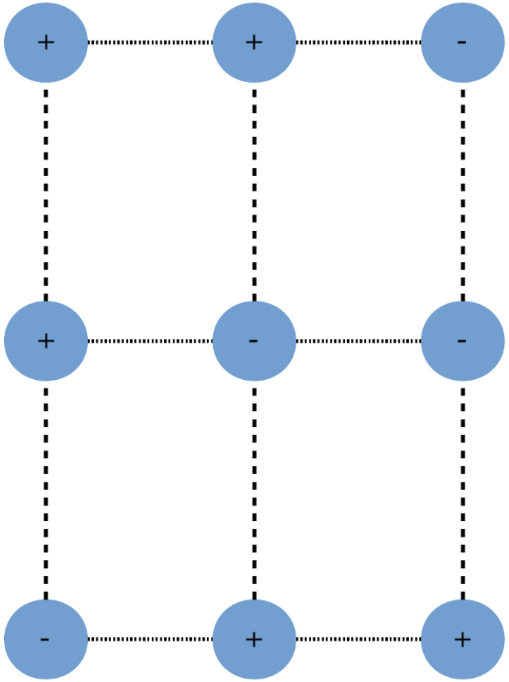
- Configuration $\sigma = \{\sigma_1, ..., \sigma_N\}$
- Energy $$E(\sigma) = E_0(\sigma) + E_1(\sigma)$$ $$= E_0(J, \sigma) - H \sum_{i=1}^{N} \sigma_i$$
- Partition function (PF) $$Z = \sum_{s} exp(-\beta E(s))$$



Basic Idea

- PF $Z_N(H,T) = \sum_{\sigma} exp(-\beta(E_0(\sigma) - H\sum_{i}\sigma_i))$
- Free energy $F = -kTln(Z)$
- Free energy per site $f(H,T) = -kT \lim_{N\to\infty} \frac{1}{N} ln(Z_N)$
- Magnetization $M(H,T) = \frac{1}{N}\langle\sigma_1 + ... + \sigma_N\rangle$

$$= -\frac{\partial}{\partial H} f(H,T)$$



Motivation [5], [11]

- Critical points (magnetization) → phase transition

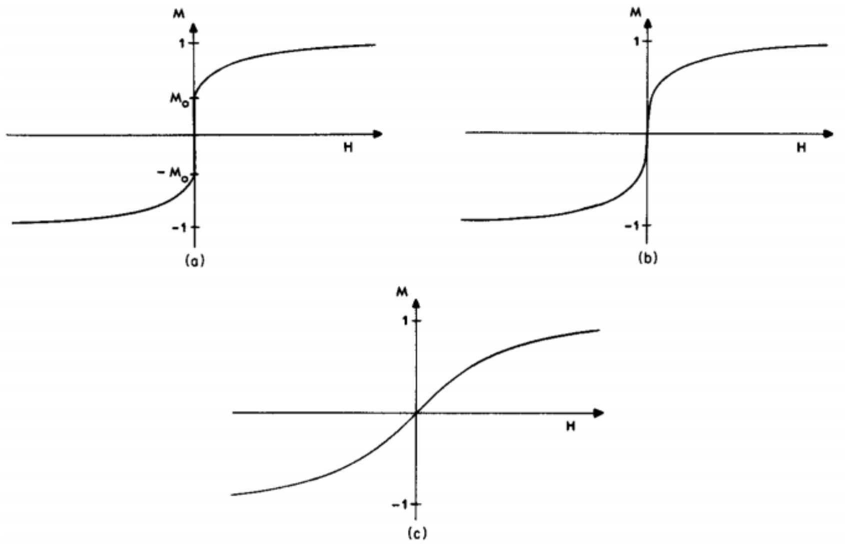


Fig. 1.1. Graphs of $M(H)$ for (a) $T < T_c$, (b) $T = T_c$, (c) $T > T_c$. [P4]

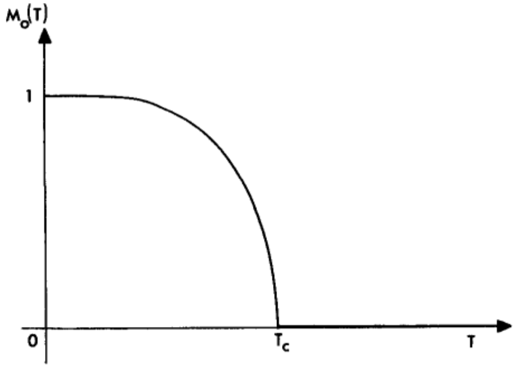
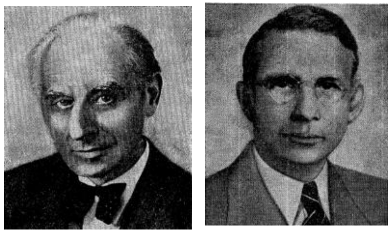


Fig. 1.3. The spontaneous magnetization M_0 as a function of temperature. [P4]

History [3], [4], [7], [11]



[P2]

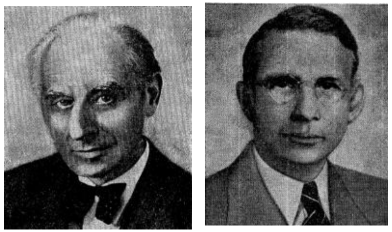
Lenz’ proposition of model

Ising’s 1D solution

1920

1925

History



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Lenz' proposition of model

Heisenberg model

Ising's 1D solution

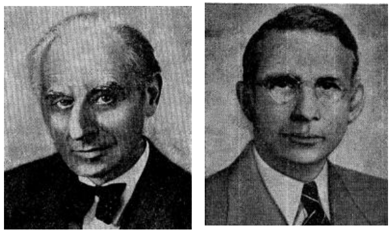
Application in different areas (1928 – 1940)

1920

1925

1928

History



[P2]

Lenz'
proposition
of model

Ising's 1D
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Heisenberg
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Application in
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Peierls'
argument
for phase
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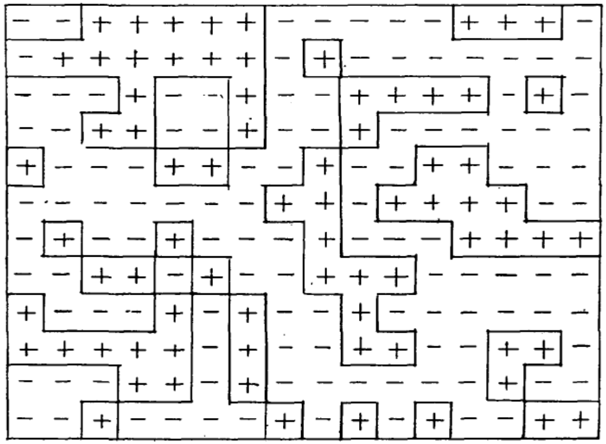
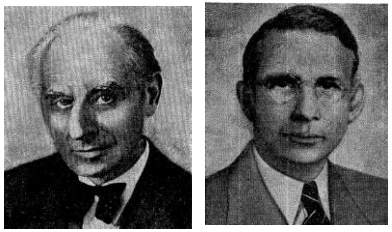


[P5]

Fig. 1. Example of boundary lines.

1920 1925 1928 1936

History



[P2]

1920	Lenz' proposition of model
1925	Ising's 1D solution
1928	Heisenberg model
	Application in different areas (1928 – 1940)
1936	Peierls' argument for phase transition
1941	Kramers& Wannier exact 2D solution
1942	Onsager exact 2D solution
	Different methods for 2D-solutions (1952 - …)

1D-Ising model – original approach [1], [7]

$$+\,+\,\underbrace{-\,-}\,+\,\underbrace{-\,-\,-\,-}\,+\,+\,+\,\underbrace{-}\,+\,+\,-\,-\,-$$

[P1]

- *N* elements (consist of + and -) $N = \nu_1 + \nu_2$
- Number of embedded ‘-’ parts: *s*
- Chain ends with + or - : δ = 0 or 1

1D-Ising model – original approach

$$+ + \underbrace{- -} + \underbrace{- - - -} + + + \underbrace{-} + + - - -$$

[P1]

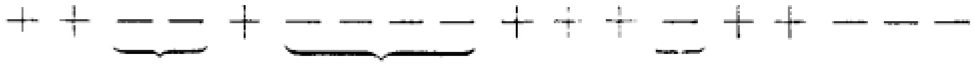
- *N* elements (consist of + and -) $N = \nu_1 + \nu_2$
- Number of embedded '-' parts: *s*
- Chain ends with + or - : *δ* = 0 or 1
- Possible configurations (for '-' in '+'-chain) $\binom{\nu_1 - 1}{s} \cdot \binom{\nu_2 - 1}{s + \delta - 1}$

Original approach

$$+\,+\,\underbrace{-\,-}\,+\,\underbrace{-\,-\,-\,-}\,+\,+\,+\,\underbrace{-}\,+\,+\,-\,-\,-$$ [P1]

- Vanishing *U* for aligned spins → else: *ε*
- For (2*s* + *δ)* '±' – zone boundaries $U = (2s + \delta) \cdot \epsilon$
- Total energy (in magnetic field *B*) $(2s + \delta)\epsilon + (\nu_2 - \nu_1)mB$

Original approach



[P1]

- Vanishing *U* for aligned spins → else: *ε*
- For (2*s* + *δ) ‘±’* – zone boundaries $U = (2s + \delta) \cdot \epsilon$
- Total energy (in magnetic field *B*) $(2s + \delta)\epsilon + (\nu_2 - \nu_1)mB$

- <u>Partition function</u>

$$Z = \sum_{\nu_1,\nu_2,s,\delta} \left[\binom{\nu_1 - 1}{s} \cdot \binom{\nu_2 - 1}{s + \delta - 1} + \binom{\nu_2 - 1}{s} \cdot \binom{\nu_1 - 1}{s + \delta - 1} \right] e^{-\beta((2s+\delta)\epsilon + (\nu_2 - \nu_1)mB)}$$

Original approach

$$+ + \underbrace{- -} + \underbrace{- - - -} + + + \underbrace{-} + + - - -$$

[P1]

- Partition function

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- Arbitrary variable *x* $F(x) = \sum_{N=0}^{\infty} Z(N) x^{\mathrm{N}}$

Original approach

$$+ \; + \; \underbrace{- \; -} \; + \; \underbrace{- \; - \; - \; -} \; + \; + \; + \; \underbrace{-} \; + \; + \; - \; - \; -$$ [P1]

- <u>Partition function</u>

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- Arbitrary variable *x* $$F(x) = \sum_{N=0}^{\infty} Z(N) x^{\mathrm{N}}$$

$$\rightarrow \quad F(x) = \frac{2x\left[\cos\alpha - (1 - \exp(-\beta\epsilon))x\right]}{1 - 2\cos\alpha \cdot x + (1 - \exp(-2\beta\epsilon))x^2}$$ with $$\alpha = \beta m B$$

Original approach

$$+ + \underbrace{- -} + \underbrace{- - - -} + + + \underbrace{-} + + - - -$$

[P1]

- Partition function

$$Z(n) = c_1 \left(\mathfrak{Cos}\,\alpha + \sqrt{\mathfrak{Sin}^2\alpha + e^{-\frac{2\varepsilon}{kT}}}\right)^n + c_2 \left(\mathfrak{Cos}\,\alpha - \sqrt{\mathfrak{Sin}^2\alpha + e^{-\frac{2\varepsilon}{kT}}}\right)^n.$$

- Magnetization

$$\mathfrak{J} = \mathfrak{m} \cdot n \cdot \frac{\mathfrak{Sin}\,\alpha}{\sqrt{\mathfrak{Sin}^2\alpha + e^{-\frac{2\varepsilon}{kT}}}}.$$

$$\alpha = \beta m B$$

Original approach

$$+\ +\ \underbrace{-\ -}\ +\ \underbrace{-\ -\ -\ -}\ +\ +\ +\ \underbrace{-}\ +\ +\ -\ -\ -$$

[P1]

- <u>Partition function</u>

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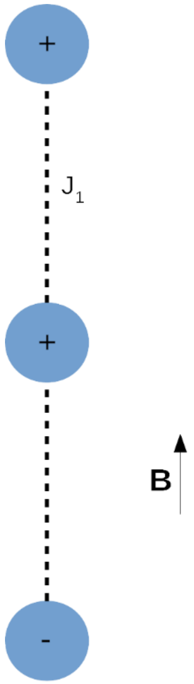
- Magnetization $\mathfrak{J} = \mathfrak{m}\cdot n\cdot\frac{\mathfrak{Sin}\,\alpha}{\sqrt{\mathfrak{Sin}^2\alpha + e^{-\frac{2\varepsilon}{kT}}}}.$ $\alpha = \beta m B$

- Spontaneous magnetization: *B* = 0 → NO!

Transfer matrix method [2], [6] - [9], [10]

- Set of spin $\frac{1}{2}$
- Bohr magneton $\mu_B = 1$
- Periodic boundary conditions

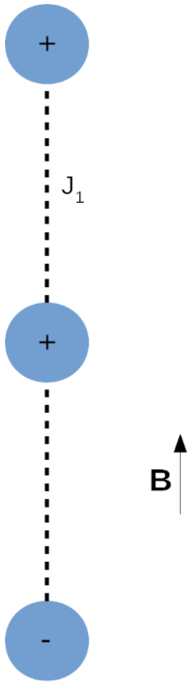


Transfer matrix method

- Set of spin $\frac{1}{2}$
- Bohr magneton $\mu_B = 1$
- Periodic boundary conditions

$$Z = \sum_{\sigma_1,\ldots,\sigma_N} \exp\left(K_1 \sum \sigma_n \sigma_{n+1}\right) \exp\left(H \sum \sigma_n\right)$$

with $K_1 = \beta J_1$, $H = \beta B$



Transfer matrix method

- Rewrite PF

$$Z = \sum_{\sigma} \left[\exp(K_1\sigma_1\sigma_2)\right]\left[\exp(0.5H(\sigma_1 + \sigma_2\right]...\left[\exp(K_1\sigma_N\sigma_1)\right]\left[\exp(0.5H(\sigma_N + \sigma_1\right]$$

Transfer matrix method

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$$\swarrow \qquad \searrow$$

$$\mathbf{V}_1 = \begin{array}{c} \begin{array}{cc} \sigma_j=+1 & \sigma_j=-1 \end{array} \\ \begin{pmatrix} e^{K_1} & e^{-K_1} \\ e^{-K_1} & e^{K_1} \end{pmatrix} \end{array} \begin{array}{c} \\ \sigma_i=+1 \\ \sigma_i=-1 \end{array} \qquad \mathbf{V}_2 = \begin{array}{c} \begin{array}{cc} \sigma_j=+1 & \sigma_j=-1 \end{array} \\ \begin{pmatrix} e^{H} & 0 \\ 0 & e^{-H} \end{pmatrix} \end{array} \begin{array}{c} \\ \sigma_i=+1 \\ \sigma_i=-1 \end{array}$$

Transfer matrix method

- Rewrite PF

$$Z = \sum_{\sigma} \left[\exp(K_1\sigma_1\sigma_2)\right]\left[\exp(0.5H(\sigma_1+\sigma_2\right]...\left[\exp(K_1\sigma_N\sigma_1)\right]\left[\exp(0.5H(\sigma_N+\sigma_1\right]$$

↙ ↘

$$\mathbf{V}_1=\begin{array}{cc|c} \sigma_j=+1 & \sigma_j=-1 & \\ \hline e^{K_1} & e^{-K_1} & \sigma_i=+1 \\ e^{-K_1} & e^{K_1} & \sigma_i=-1 \end{array} \qquad \mathbf{V}_2=\begin{array}{cc|c} \sigma_j=+1 & \sigma_j=-1 & \\ \hline e^{H} & 0 & \sigma_i=+1 \\ 0 & e^{-H} & \sigma_i=-1 \end{array}$$

- PF in terms of transfer matrices

$$Z = \mathrm{tr}(V_1V_2)^N$$
$$= \mathrm{tr}(V_2^{\frac{1}{2}}V_1V_2^{\frac{1}{2}})^N = \mathrm{tr}V^N$$

Transfer matrix method

- Eigenvalues of V : $\Lambda_1 > \Lambda_2$

$$Z = \Lambda_1^N + \Lambda_2^N = \Lambda_1^N (1 + (\Lambda_2/\Lambda_1)^N)$$

Transfer matrix method

- Eigenvalues of $V : \Lambda_1 > \Lambda_2$

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- For $N \to \infty$

➡ determining largest eigenvalue

of transfer matrix yields free energy

- Eigenvalues

$$\Lambda_{1,2} = e^{K_1} \cosh(H) \pm \sqrt{e^{2K} \sinh^2(H) + e^{-2K}}$$

Transfer matrix method

- Eigenvalues of $V: \Lambda_1 > \Lambda_2$

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- Eigenvalues

$$\Lambda_{1,2} = e^{K_1} \cosh(H) \pm \sqrt{e^{2K} \sinh^2(H) + e^{-2K}}$$

- Magnetization $$M(H,T) = \frac{e^{K_1} \sinh(H)}{\sqrt{e^{2K_1} \sinh^2(H) + e^{-2K_1}}}$$

Transfer matrix method

- Decomposition of V in Pauli matrices τ^i

$$\mathbf{V}_1 = \left(\begin{array}{c|c} e^{K_1} & e^{-K_1} \\ \hline e^{-K_1} & e^{K_1} \end{array}\right) \qquad \mathbf{V}_2 = \left(\begin{array}{c|c} e^{H} & 0 \\ \hline 0 & e^{-H} \end{array}\right)$$

$$V_1 = e^{K_1} \cdot 1 + e^{-K_1} \tau^x \qquad V_2 = 1 \cdot \cosh(H) + \tau^z \sinh(H)$$

- For all Pauli matrices $\exp(a\tau^i) = 1 \cdot \cosh(a) + \tau^i \sinh(a)$

$$V_1 = (2\sinh(2K_1))^{\frac{1}{2}} \exp(K_1^* \tau^x) \qquad V_2 = \exp(H\tau^z)$$

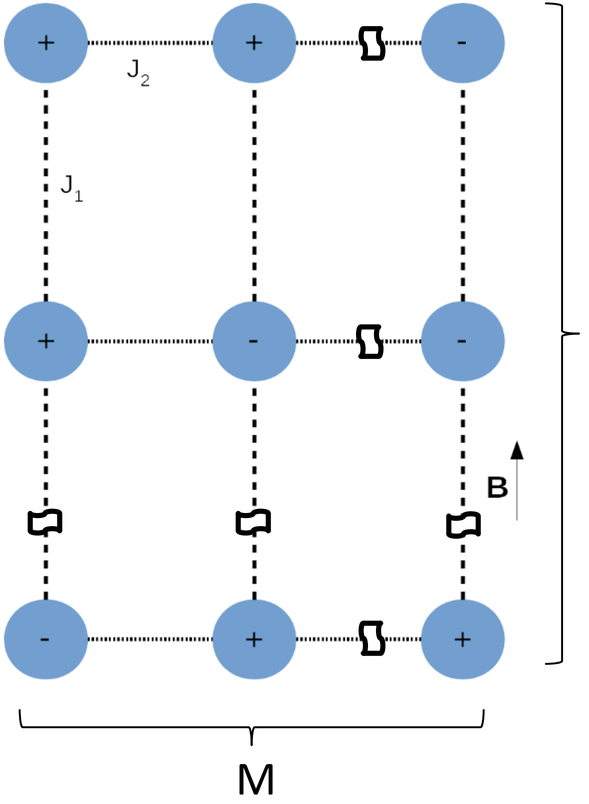
with $\tanh(K_1^*) \equiv e^{-2K_1}$ and $\sinh(2K_1)\sinh(2K_1^*) \equiv 1$

2D-Ising model - transfer matrix method [2], [6] - [9], [10]

- Rectangular lattice *MxN* (*columns* x *rows*)
- Sum now over 2^M configurations of each row

$$V_1 = (2\sinh(2K_1))^{\frac{M}{2}} \exp(K_1^* \sum \tau_m^x)$$

$$V_2 = \exp(K_2 \sum \tau_m^z \tau_{m+1}^z + H \sum \tau_m^z)$$



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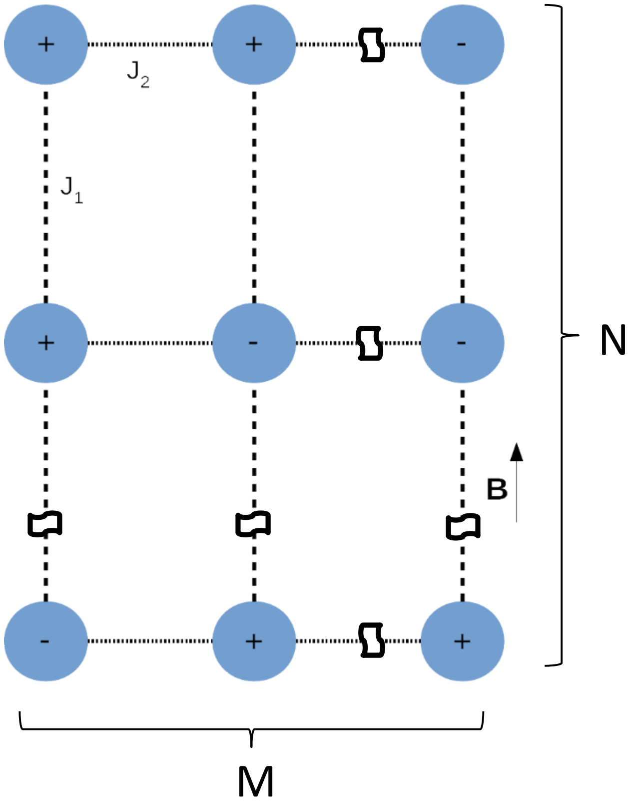
$$\swarrow \qquad \searrow$$

$$V_2 = \exp(K_2 \sum \tau_m^z \tau_{m+1}^z) \; V_3 = \exp(H \sum \tau_m^z)$$

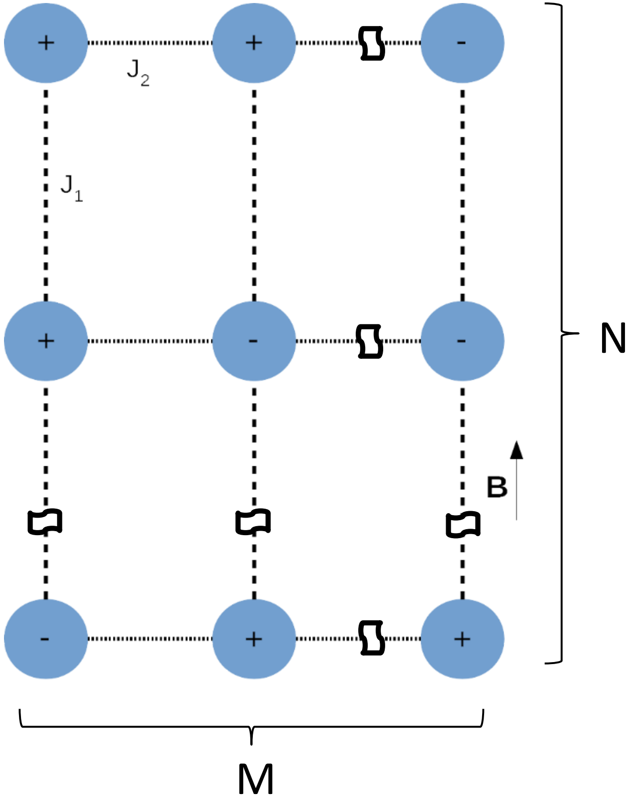


Transfer matrix method

- Matrices now 2^M x 2^M

$$\tau^i_m = 1 \times \cdots \times 1 \times \tau^i \times 1 \times \cdots \times 1$$

(with τ^i at *m*th-position)



Transfer matrix method

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$$\tau^i_m = 1 \times \cdots \times 1 \times \tau^i \times 1 \times \cdots \times 1$$

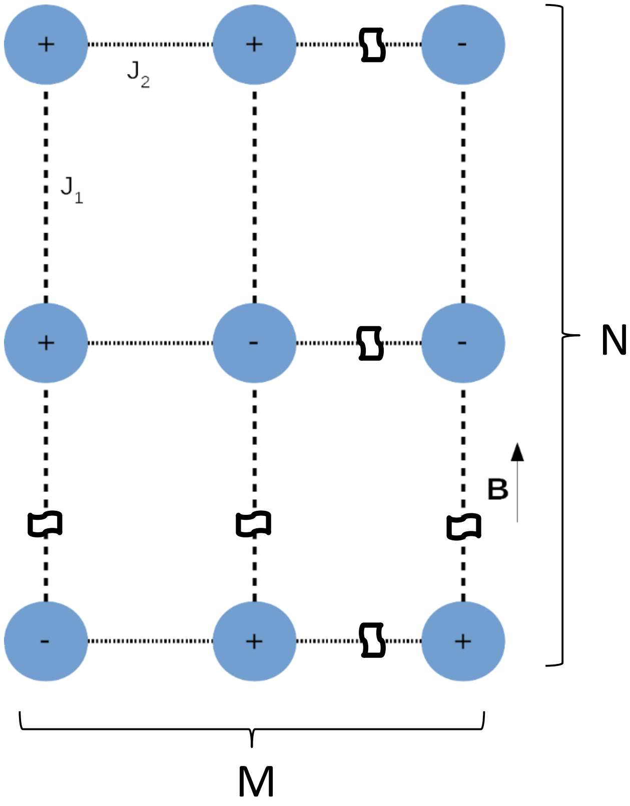
(with τ^i at *m*th-position)

- Direct product

$$\langle \beta b \,|\, \mathfrak{A} \times \mathbf{A} \,|\, \alpha a \rangle = \langle \beta \,|\, \mathfrak{A} \,|\, \alpha \rangle \langle b \,|\, \mathbf{A} \,|\, a \rangle$$

- Partition function

$$Z = tr\left[(V_2V_3)^{\frac{1}{2}} V_1 (V_2V_3)^{\frac{1}{2}}\right]^N$$



Onsagers' exact solution [10]

- Free energy *f*

$$-\beta f = \ln(2) + \frac{1}{8\pi^2}\int_0^{2\pi} d\theta_1 \int_0^{2\pi} d\theta_2 ln\left[\cosh(2\beta J_1)\cosh(2\beta J_2) - \sinh(2\beta J_1)\cos(\theta_1) - \sinh(2\beta J_2)\cos(\theta_2)\right]$$

- Critical temperature

$$\sinh\left(\frac{2J_1}{kT_c}\right)\sinh\left(\frac{2J_2}{kT_c}\right) = 1$$

- Critical temperature for square lattice

$$T_C = \frac{2J}{k\ln(1+\sqrt{2})}$$

Metropolis algorithm [V1‘]

[V1]

Achievements of the Ising model [4], [5], [7]

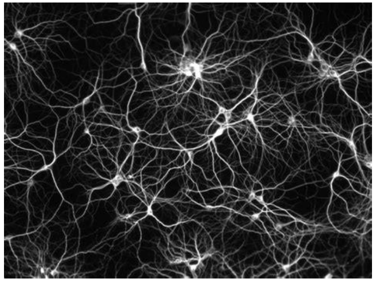
- Exactly soluble (1D and 2D) → testing new models
- Representation of many physico-chemical systems
- Connecting different fields in science, e.g.:

  order-disorder transformations in alloys,

  magnetic Curie points,

  properties of critical gas-liquid phenomena,

  neuroscience



[P3]

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Picture References

[P1] E. Ising (1925). *Beitrag zur Theorie des Ferromagnetismus*, Z. Physik 31, 253

[P2] S.G. Brush (1967). *History of the Lenz-Ising model*, Rev. Mod. Phys. 39, 883

[P3] http://wccftech.com/scientists-artificial-neurons-mimics-human-brain-cells/

[P5] R. Peierls (1936). *Ising‘s model of ferromagnetism*, Proc. Cambridge Phil. Soc., Band 32, 477

Video References

[V1] https://www.youtube.com/watch?v=wobhrL3IGa0

[V2‘] https://github.com/CodingPhysics/Ising