Thermodynamic Magnetic Simulations

Ising Model with Metropolis Algorithm

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Based on *A Survey of Computational Physics* by Landau, Páez, & Bordeianu

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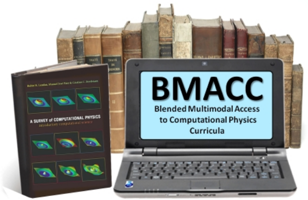
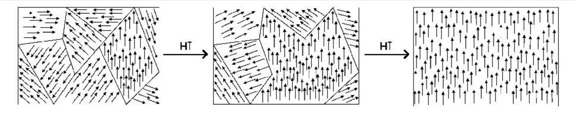
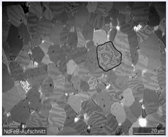
Course: **Computational Physics II**



Problem: Explain Thermal Behavior of Ferromagnets

What are Magnets and How Do They Behave?

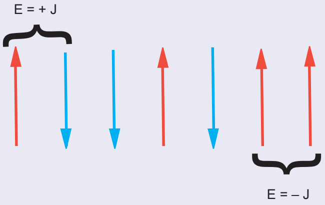




- Ferromagnets $= \sum$ finite domains
- Domain: all atoms' spins aligned
- External $\vec{B}$: align domains $\Rightarrow$ magnetized
- $T \uparrow$: $\sum$ magnetism $\downarrow$ (spins flip?)
- @ T_{curie}: phase transition, $\vec{M} = 0$
- Explain more than usual

Ising Model: N Magnetic Dipoles on Linear Chain

Constrained Many Body Quantum System

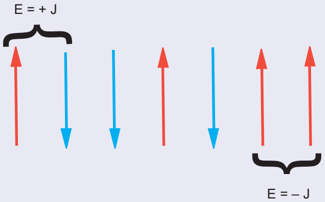


- Same model 2-D, 3-D
- Fixed $\Rightarrow$ no movements
- Spin dynamics
- Particle i, spin
- $s_i \equiv s_{z,i} = \pm\frac{1}{2}$
- Ψ: N spin values

$$|\alpha_j\rangle = |s_1, s_2, \ldots, s_N\rangle = \left\{\pm\frac{1}{2}, \pm\frac{1}{2}, \ldots\right\}, \quad j = 1, \ldots, 2^N$$

Ising Model Continued

Quantum Interaction of N Magnetic Dipoles



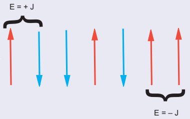
$$V_i = -J\vec{s}_i \cdot \vec{s}_{i+1} - g\mu_b\, \vec{s}_i \cdot \vec{B}$$

- $s_i = \uparrow, \downarrow \;\Rightarrow 2^N$ states
- Fixed $\;\Rightarrow$ no exchange
- Energy: $\vec{\mu} \cdot \vec{\mu} + \vec{\mu} \cdot \vec{B}$
- J = exchange energy

- $J > 0$: ferromagnet $\uparrow\uparrow\uparrow$
- $J < 0$: antiferromagnet $\uparrow\downarrow\uparrow\downarrow$
- g = gyromagnetic ratio
- $\vec{J} = g\vec{\mu}$
- $\mu_b = e\hbar/(2m_e c)$

Many Body Problem ($N \geq 2, 3$ Unsolved)

Beyond $N = 2$, 3 Use Statistics, Approximations



$$E_{\alpha_k} = -J \sum_{i=1}^{N-1} s_i s_{i+1} - B\mu_b \sum_{i=1}^{N} s_i$$

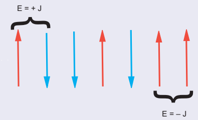
- $2^N \rightarrow$ large ($2^{20} > 10^6$)
- 10^{23}: hah!
- $B_{ext} \rightarrow 0 \Rightarrow$ no direction
- $\Rightarrow < \vec{M} >= 0$
- Yet spins aligned??
- Spontaneous reversal

- Not equilibrium approach
- Curie Temperature: $\vec{M}(T > T_c) \equiv 0$
- $T < T_c$: quantum macroscopic order
- 1D: no phase transition

Statistical Mechanics (Theory)

Microscopic Origin of Thermodynamics

- Basis: all configurations $<$ constraints possible
- *Microcanonical Ensemble*: energy fixed
- *Canonical Ensemble*: (here) $T,\ V,\ N$ fixed, not E
- "At temperature T": equilibrium $\langle E \rangle \propto T$
- Equilibrium $\not\Rightarrow$ static $\Rightarrow$ continual random fluctuates
- Canonical ensemble: E_α vary via Boltzmann (k_B):



$$\mathcal{P}(E_\alpha, T) = \frac{e^{-E_\alpha / k_B T}}{Z(T)}$$

$$Z(T) = \sum_\alpha e^{-E_\alpha / k_B T}$$

- Sum: individual states, not $g(E_\alpha)$ weighted sum

Analytic Solutions $N \rightarrow \infty$ Ising Model

1-D Ising

$$U = \langle E \rangle \tag{1}$$

$$\frac{U}{J} = -N \tanh \frac{J}{k_B T} = -N \frac{e^{J/k_B T} - e^{-J/k_B T}}{e^{J/k_B T} + e^{-J/k_B T}} = \begin{cases} N, & k_B T \rightarrow 0, \\ 0, & k_B T \rightarrow \infty \end{cases} \tag{2}$$

$$M(k_B T) = \frac{N e^{J/k_B T} \sinh(B/k_B T)}{\sqrt{e^{2J/k_B T} \sinh^2(B/k_B T) + e^{-2J/k_B T}}}. \tag{3}$$

2-D Ising

$$\mathcal{M}(T) = \begin{cases} 0, & T > T_c \\ \frac{(1+z^2)^{1/4}(1-6z^2+z^4)^{1/8}}{\sqrt{1-z^2}}, & T < T_c, \end{cases} \tag{4}$$

$$kT_c \simeq 2.269185J, \quad z = e^{-2J/k_B T}, \tag{5}$$

Metropolis Algorithm (A Top 10 Pick)

Basic Concepts (Mystery That It Works)

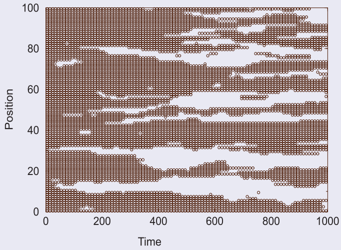
- Boltzmann $\not\Rightarrow$ system remain lowest E state
- Boltzmann $\Rightarrow$ higher E less likely than lower E
- $T \rightarrow 0$: only lowest E
- Finite T: $\Delta E \sim k_B T$ fluctuations $\sim$ equilibrium
- Metropolis, Rosenbluth, Teller & Teller: n transport
- Clever way improve Monte Carlo averages
- Simulates thermal equilibrium fluctuations
- Randomly change spins, $\langle$follows$\rangle \simeq$ Boltzmann
- Combo: variance reduction & von Neumann rejection

Metropolis Algorithm Implementation

Number of Steps, Multiple Paths to Equilibrium Configuration

1. Start: fixed T, arbitrary $\alpha_k = \{s_1, s_2, \ldots, s_N\}$, E_{α_k}
2. Trial: flip random spin(s), calculate E_{trial}
3. If $E_{trial} \leq E_{\alpha_k}$, accept: $\alpha_{k+1} = \alpha_{trial}$
4. If $E_{trial} > E_{\alpha_k}$, accept + relative probable $\mathcal{R} = e^{-\frac{\Delta E}{k_B T}}$:
   - Choose uniform $0 \leq r_i \leq 1$
   - Set $\alpha_{k+1} = \begin{cases} \alpha_{trial}, & \text{if } \mathcal{R} \geq r_j \text{ (accept)}, \\ \alpha_k, & \text{if } \mathcal{R} < r_j \text{ (reject)}. \end{cases}$
5. Iterate, equilibrate (wait $\simeq 10N$)
6. Physics = fluctuations $\to M(T)$, $U(T)$
7. Change T, repeat

Metropolis Algorithm Implementation (`IsingViz.py`)

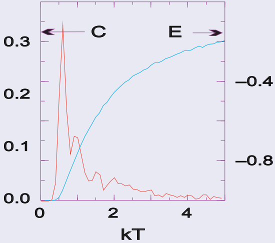


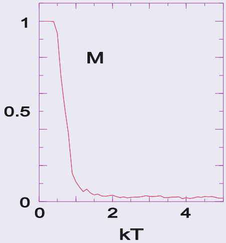
- Hot start: random
- Cold start: parallel, anti
- $> 10N$ iterates no matter
- More averages better
- Data structure = `s[N]`
- Print $+$, $-$ ea site
- Periodic BC

- 1st $J = k_B T = 1$, $N \leq 20$
- Watch equilibrate: Δ starts
- Large flucts: $\uparrow T$, $\downarrow N$
- Large $k_B T$: instabilities
- Small $k_B T$: slow equilibrate
- Domain formation & total E ($E > 0$: $\uparrow\downarrow$, $\downarrow\uparrow$)

Calculate Thermodynamic Properties

Average in Equilibrium 100 spins





$$E_{\alpha_j} = -J \sum_{i=1}^{N-1} s_i s_{i+1}, \qquad \mathcal{M}_j = \sum_{i=1}^{N} s_i, \qquad C_{simple} = \frac{1}{N}\frac{d\langle E\rangle}{dT}$$

- $\vec{M}(k_b T \to \infty) \to 0$
- $\vec{M}(k_b T \to 0) \to N/2$

Get to Work!