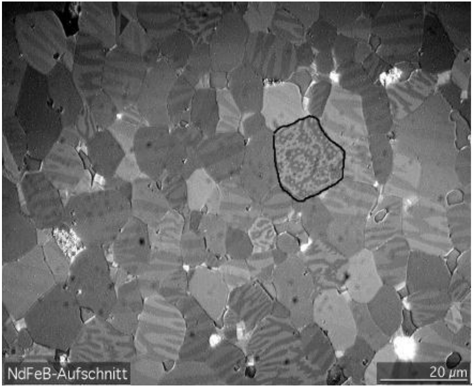
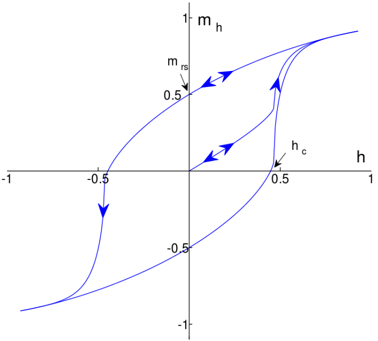
Ferromagnets and the Ising Model

MSE 421 - Ceriotti

Ferromagnetic materials

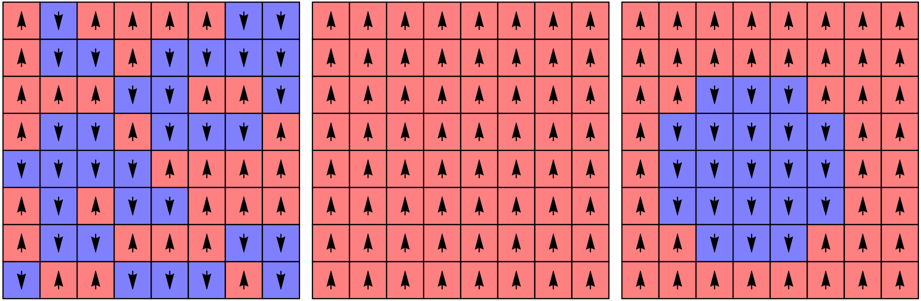
- Recall that for a paramagnetic material, there is no magnetization in the absence of an external field
- How can we explain ferromagnetic behavior, where there is a residual magnetization at zero field?
- How can we explain hysteresis?





Spins on a lattice

- The microscopic model is similar to that of a paramagnet. Each atom carries a magnetic moment, that can orient itself relative to a magnetic field
- Crucially, spins interact with each other $\rightarrow Q \neq q^N$!!



E/site : 0.1875
μ/site : –0.03125

E/site : –2.000
μ/site : 1.000

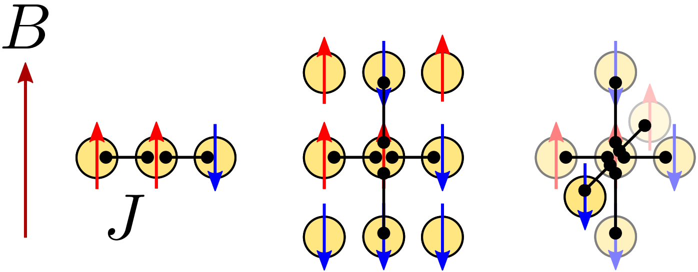
E/site : –1.375
μ/site : 0.3438

The Heisenberg Hamiltonian

- Simplest possible model of spin interactions (AKA Ising model). Each site associated with $s_j = \pm 1$, first-neighbor interactions

$$H = -\mu_B B \sum_i s_i - \frac{1}{2} J \sum_i \sum_{j \in \mathcal{N}_i} s_i s_j$$

- The behavior depends dramatically on the dimensionality of the lattice



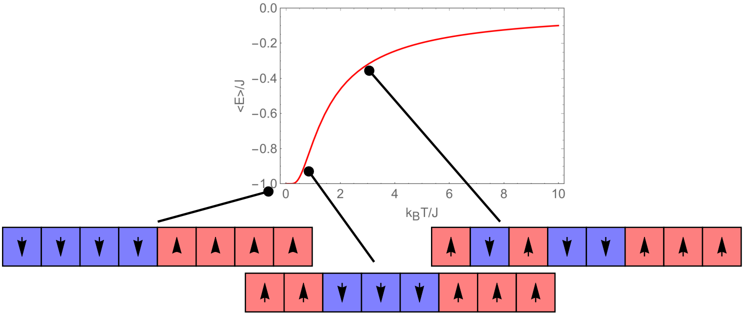
Ising model in 1D

- Consider the case without a magnetic field. We can make the change of variables $s_i s_{i+1} \rightarrow s_i'$

$$Q = \sum_{\{s\}} \prod_i e^{\beta J s_i s_{i+1}} = \sum_{\{s'\}} \prod_i e^{\beta J s_i'} = \prod_i \left(e^{\beta J} + e^{-\beta J} \right) = \left[2 \cosh \beta J \right]^N$$

- Average energy

$$-\frac{\partial \ln Q}{\partial \beta} = -NJ \frac{e^{J/k_B T} - e^{-J/k_B T}}{e^{J/k_B T} + e^{-J/k_B T}} = -NJ \tanh \beta J$$

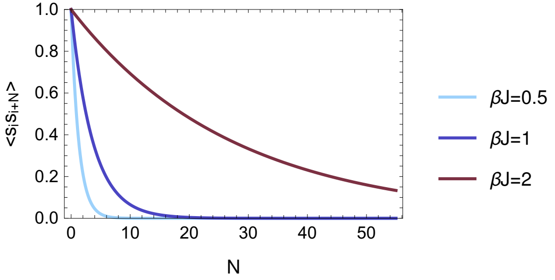


Spin correlations

- $\langle s_i s_{i+N} \rangle$ measures the probability that two spins separated by N sites have the same orientation
- How quickly do spin fluctuations decay? Substitution $s_i s_{i+1} \rightarrow s'_i$

$$\langle s_i s_{i+N} \rangle = \frac{\sum_{\{\mathbf{s}\}_N} s_1 s_N \prod_i e^{\beta J s_i s_{i+1}}}{\sum_{\{\mathbf{s}\}_N} \prod_i e^{\beta J s_i s_{i+1}}} = \frac{\sum_{\{\mathbf{s}'\}_N} \prod_i s'_i e^{\beta J s'_i}}{\sum_{\{\mathbf{s}'\}_N} \prod_i e^{\beta J s'_i}} = [\tanh \beta J]^N$$

- Exponential decay of correlations. No phase transition except at $T = 0$



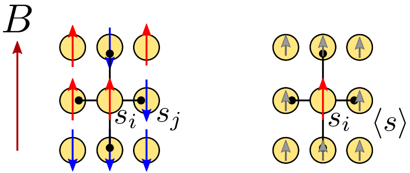
2D and above: mean field model

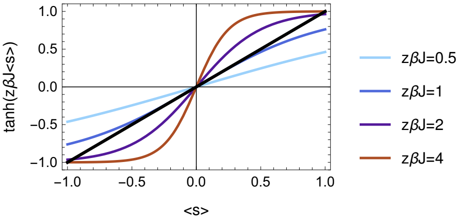
- The 2D case is much harder. A (nobel-prize-worthy) solution exists due to Lars Onsager. How do we proceed?
- Consider the substitution $s_i \to \langle s \rangle + \delta s_i$. Neglect the quadratic term $\delta s_i \delta s_j$ $\to$ partition function can be factorized, probability depends on mean spin $\langle s \rangle$ and the number of neighbors z

$$-H_{MF} = -\frac{N}{2} zJ \langle s \rangle^2 + \sum_i \mu_B B s_i + zJ \langle s \rangle s_i, \qquad P(s_i) \propto e^{\beta[\mu_B B + zJ\langle s \rangle] s_i}$$

- Self-consistent equation for $\langle s \rangle$

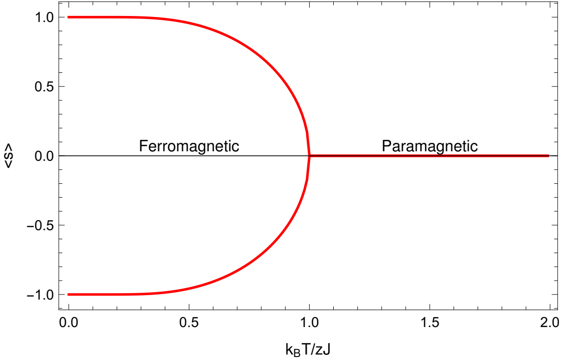
$$\langle s \rangle = \sum_{\pm 1} s_i P(s_i) = \tanh\left[\beta \mu_B B + zJ\beta \langle s \rangle\right]$$





Phase transitions in the Ising model

- For $B = 0$, $\langle s \rangle = \tanh\left[\beta\mu_B B + zJ\beta \langle s \rangle\right]$ has two solutions for $k_B T/zJ < 1$
- For $k_B T/zJ > 1$, only one solution $\langle s \rangle = 0$
- The system has a phase transition at $T_c = zJ/k_B$



Magnetization

- Start by considering the partition function

$$Q = q^N = \left[2e^{-\frac{\beta zJ\langle s\rangle^2}{2}}\cosh\left(\beta\mu_B B + \beta zJ\langle s\rangle\right)\right]^N$$

- What is the mean magnetization?

$$\langle M\rangle = \mu_B N\langle s\rangle = \frac{1}{\beta}\frac{\partial \ln Q}{\partial B} = N\mu_B \tanh\left[\beta\mu_B B + \beta zJ\langle s\rangle\right]$$

- At high temperature $\langle s\rangle \approx 0$, $\mathcal{O}(B)$ expansion $\rightarrow$ paramagnet!

$$\langle m\rangle = \langle M\rangle / N = \mu_B\langle s\rangle = \frac{\mu_B^2 B}{k_B T}$$

- Close to the critical point, and for $B = 0$, we can take a series expansion for $\tanh x \approx x - \frac{1}{3}x^3$. Define reduced temperature $t = \frac{T - T_c}{T_c}$

$$\langle s\rangle^2 = 3\left(1+t\right)^2\left(-t\right) \approx -3t$$

- The order parameter grows as $t^{1/2}$ close to T_c. This is an example of a *critical exponent*, describing the behavior close to a phase transition

Susceptibility

- The response to a magnetic field is given by the susceptibility $\chi = \partial \langle m \rangle / \partial B$. Take first order expansion in B

$$\chi = \beta \mu_B^2 + \frac{T_c}{T}\chi - \left(\frac{T_c}{T\mu_B}\right)^3 \chi \langle m \rangle^2$$

- For $T \gtrsim T_c$, $\langle m \rangle \approx 0$

$$\chi \approx \frac{\beta\mu_B^2}{1-\frac{T_c}{T}} \approx \frac{\beta\mu_B^2}{t}$$

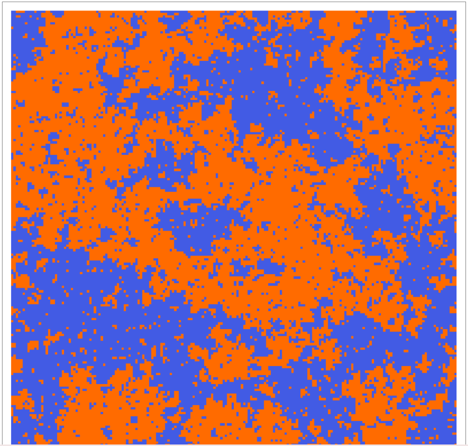
- For $T \lesssim T_c$,we also retain the $\mathcal{O}\left(\langle m \rangle^3\right)$ term

$$\chi \approx \frac{\beta\mu_B^2}{1-\frac{T_c}{T}+3\left(\frac{T}{T_c}\right)^3\left(\frac{T_c}{T}-1\right)\left(\frac{T_c}{T\mu_B}\right)^3} = \frac{\beta\mu_B^2}{1-\frac{T_c}{T}+3\left(\frac{T_c}{T}-1\right)} \approx -\frac{\beta\mu_B^2}{2t}$$

- Critical exponent is 1

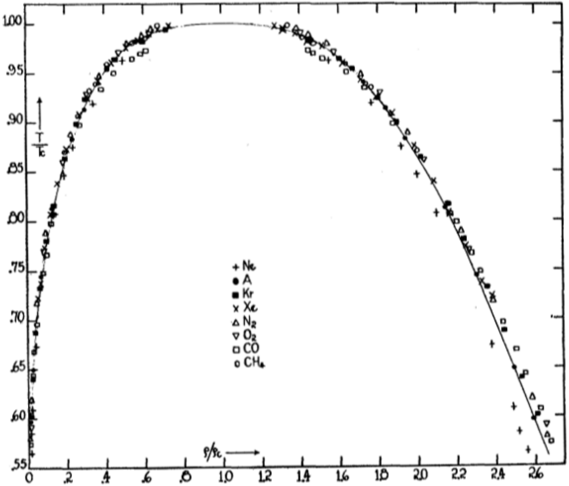
Limitations of the mean-field model

- Predicts a finite-temperature phase transition for the 1D Ising model. Overestimation of the transition temperature in higher dimensions
- Finite extent of susceptibility and heat capacity at non-zero field
- No trace of hysteresis, or barriers to the formation of disorder
- Several better (but much more complex) approximations available. Alternative: explicit simulations of the Ising model (see lab!)



Universality of critical exponents

- Observation: very different systems shows remarkably similar asymptotic behavior in the vicinity of a critical point - **universality**
- Can we explain (handwavingly) the phenomenon based on what we know?



Mapping on the Ising model

- Example: a lattice gas (e.g. adsorbates on a surface, vacancies, ...) - more in the exercises!
- Hamiltonian describes small cells that have either 0 or 1 molecules. Chemical potential is μ_B, bond energy is ϵ

$$H = -\mu_B \sum_i n_i - \frac{\epsilon}{2} \sum_{i,j \in N_i} n_i n_j$$

- Can be mapped on a Ising model with the substitution $n_i = (s_i + 1)/2$

$$H = C - \mu_B B \sum_i s_i - \frac{J}{2} \sum_{i,j \in N_i} s_i s_j, \qquad \mu_B B = \frac{\mu_B}{2} + z\frac{\epsilon}{4}, J = \frac{\epsilon}{4}$$