Statistical Mechanics
E0415

2020, summary 4
Ising model, 2nd order phase transitions

Take home 3

This lecture looks at the classical measures of correlations and their decay. We shall get back to these topics later on, but you should read through the chapter and think of conditional probabilities. Read first the Chapter and check then the lecture slides again.

The take home consists of answering to the following questions:

Give an example of X and Y that are correlated but there is no causal relation (X because of Y or X because of Y happened before) between them.

Take a (time) series of the binary kind 0110110011000111.... (or subtract -1/2 from all the values so that the average might become zero). When would this be correlated?

Take instead a series like this: ...00001111111(...)111000.... This is clearly not a random one. Now start tossing a coin (0/1) and replace according to each toss one of the values with the new one. Does this correspond to the Onsager hypothesis and why? If the coin is biased, does the process relate to linear response?

As a final remark, try playing the game found at `https://www.expunctis.com/2019/03/07/Not-so-random.html`. How random were you able to be?

Give an example of X and Y that are correlated but there is no causal relation:

"X: Many people are wearing a jacket in Finland. Y: The leaves are falling off the trees in Finland.“

"A classic example to this would be the correlation between the number of pirates and the global warming.“

Take a (time) series of the binary kind...:

"For a random binary series Xn, Corr(Xn,Xn+k)=E[XnXn+k]−E[Xn]E[Xn+k]. So if Xn and Xn+k are independent, Corr(Xn,Xn+k)=0"

“-- would be correlated if for some index i in the following indices i+k would have on average over 50% chance of being the same value as i."

Take…

Take instead a series like this...:

"The Onsager hypothesis states that a spontaneous deviation from the equilibrium decays according to the same laws as one that has been produced artificially. I think a coin toss and its effect on a non-random series corresponds to the Onsager hypothesis, since the coin toss is a spontaneous deviation. It could be argued that the deviation decays in a similar fashion than if the series was just randomized artificially. With a biased coin, the process relates to linear response, since the series experiences a kick into a direction or another depending on the coin bias. The series responds by shifting towards one direction.

"As the number of coin flips goes to infinity, the system becomes random and the correlation becomes zero. As the process goes on, the size of the 'islands' decays. According to the Onsager hypothesis the decay process of the islands would be the same as the decay in correlation (or vise-versa). If the coin toss is biased, the system can be thought as if having a force acting in one direction, analogously to linear system."

As a final remark, try playing the game..:

ABC of phase transitions

Today's main topics:

- The paradigmatic statistical mechanics model: the Ising model
- How to solve statistical mechanics on the computer – yet another connection to stochastics (of/or Markov chains)
- Coarse-grain the Ising: simplest Ginzburg-Landau theory, the phase transition in GL.

Material: Sethna, Chaikin-Lubensky, Principles of Condensed Matter Physics, Ch 4 (start) and Ch 10 (early part).

Meet the Ising model

- Lattice model, with Hamiltonian

$$\mathcal{H} = -\sum_{\langle ij \rangle} J s_i s_j - H \sum_i s_i.$$

- These details dictate the physics: J (coupling), H (external field), sum over (NN) interactions, geometry.
- Sign of J: (anti)ferromagnetic. Trees, 1D (solvable), 2D (barely solvable), 3D (not solvable).
- Add disorder (RF [H], RB (J), SG (J)), make J long-ranged, AF in a triangular lattice (frustration)….

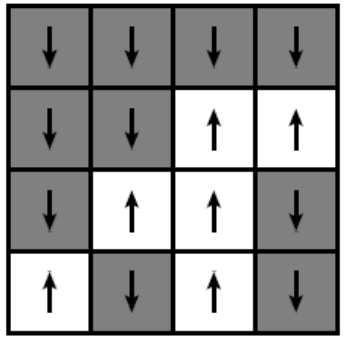


Fig. 8.1 The 2D square-lattice Ising model. It is traditional to denote the values $s_i = \pm 1$ as up and down, or as two different colors.

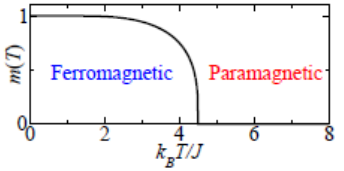


Fig. 8.2 Ising magnetization. The magnetization $m(T)$ per spin for the 3D cubic lattice Ising model. At low temperatures there is a net magnetization, which vanishes at temperatures $T > T_c \approx 4.5$.

Ising model: (some) uses

Magnetism (parameters from microscopic detail!).

Binary alloys: understand the energy from the atomistic configuration (NN, NNN…).

Liquid-gas transition: what happens in the phase diagram close to the critical point (liquid-gas).

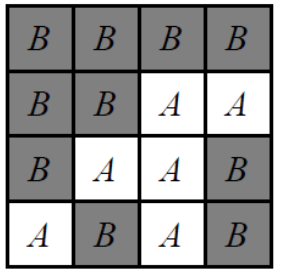


Fig. 8.3 The Ising model as a binary alloy. Atoms in crystals naturally sit on a lattice. The atoms in alloys are made up of different elements (here, types A and B) which can arrange in many configurations on the lattice.

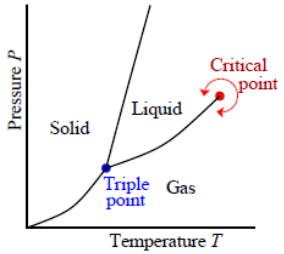


Fig. 8.4 P–T **phase diagram** for a typical material. The solid–liquid phase boundary corresponds to a change in symmetry, and cannot end. The liquid–gas phase boundary typically does end; one can go continuously from the liquid phase to the gas phase by increasing the pressure above P_c, increasing the temperature above T_c, and then lowering the pressure again.

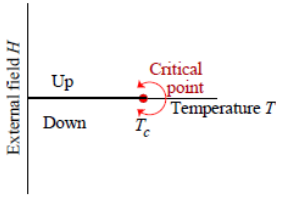


Fig. 8.5 H–T **phase diagram for the Ising model.** Below the critical temperature T_c, there is an an up-spin and a down-spin 'phase' separated by a jump in magnetization at $H = 0$. Above T_c the behavior is smooth as a function of H.

How to solve the Ising model?

Emulate the thermal evolution on a computer: Heat Bath algorithm.

Pick a spin (at random).

Compute the cost in energy for having it up/down $\Delta E_{up/down}$.

Pick the direction at random using the right Boltzmann weights.

(This means we do a Markov Chain over the spin states).

Advanced numerical methods:

Cluster algorithms…

Parallel tempering…

Ground-state methods for disordered systems (low temperatures: unique ground state for each system)…

Special computers (!).

Markov chains/fields (in general)

Properties of (memoryless) processes for the evolution of the occupation probabilities, $p(n)_\alpha$.

Require a steady-state, and conservation of probability.

Ergodic (finite convergence time) chains have a single steady-state (Frobenius-Perron theorem).

Detailed balance: convergence assured.

- **Time evolution.** The probability vector at step $n+1$ is

$$\boldsymbol{\rho}_\beta(n+1) = \sum_\alpha P_{\beta\alpha}\boldsymbol{\rho}_\alpha(n), \qquad \boldsymbol{\rho}(n+1) = P \cdot \boldsymbol{\rho}(n). \tag{8.6}$$

- **Positivity.** The matrix elements are probabilities, so

$$0 \leq P_{\beta\alpha} \leq 1. \tag{8.7}$$

- **Conservation of probability.** The state α must go somewhere, so

$$\sum_\beta P_{\beta\alpha} = 1. \tag{8.8}$$

- **Not symmetric!** Typically $P_{\beta\alpha} \neq P_{\alpha\beta}$.

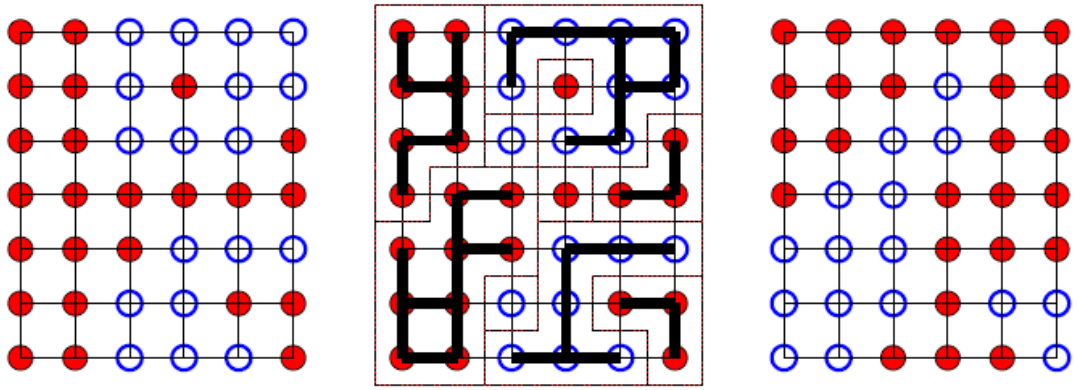
$$P_{\alpha\beta}\rho^*_\beta = P_{\beta\alpha}\rho^*_\alpha$$

Example #1 of cluster algorithms

- Swendsen and Wang 1989 [PRL 56 (87), 86]: update clusters not single spins.
- Does this give the correct thermodynamics?

Beginning with an arbitary configuration s_i, one SW cluster update cycle is:

1. Inspect all nn-states s_i, s_j. If $s_i = s_j$, create a bond between sites i, j with probability $p = 1 - \exp(-2\beta)$ (otherwise no bond).
2. Construct clusters = sets of points connected by bonds.
3. Set each cluster to a *random* value ± 1.



Thx to K. Rummukainen, HY

Check it out

Showing that the SW algorithm exhibits detailed balance (between A and B) follows essentially from the fact that the intermediate ”C” after the flip is arbitary and compatible with both.

Is this a valid update? It satisfies

a) ergodicity (obvious)

b) detailed balance: $\frac{P(A \mapsto B)}{P(B \mapsto A)} = \exp -\beta(E_B - E_A)$?

Proof: consider $A \mapsto \mathcal{C} \mapsto B$, where $\mathcal{C}$ is some bond configuration compatible with both A and B. Since the clusters in $\mathcal{C}$ are independent, $P(\mathcal{C} \mapsto A) = P(\mathcal{C} \mapsto B) = 1/2^{N_c}$.

Now,

$$\frac{P(A \mapsto \mathcal{C})}{P(B \mapsto \mathcal{C})} = \frac{p^b\,(1-p)^{d_A}}{p^b\,(1-p)^{d_B}} = \exp[-\beta(E_B - E_A)]$$

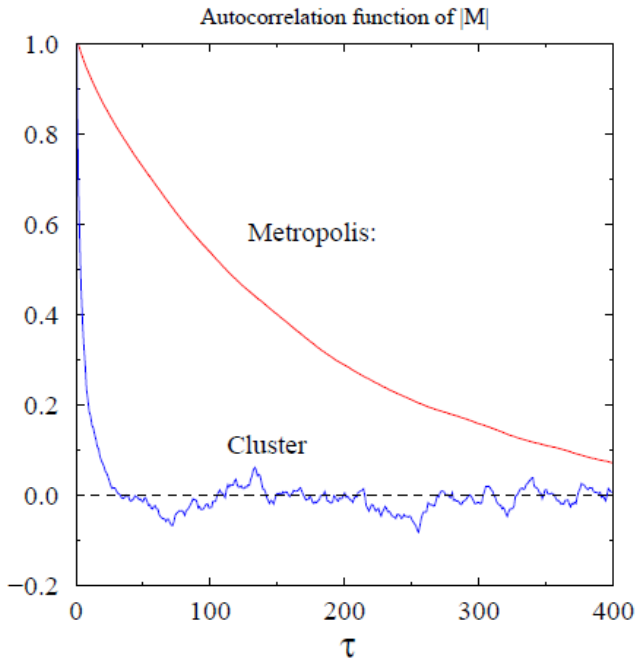
where $d_{A,B}$ are the numbers of similar nn-states which are not connected by a bond. The last step comes from $E_A = \text{dim} \times V - 2(b + d_A)$. Thus $A \mapsto \mathcal{C} \mapsto B$ and $B \mapsto \mathcal{C} \mapsto A$ satisfy detailed balance for arbitrary $\mathcal{C}$, and the total transition probabilities $A \mapsto B$, $B \mapsto A$ must do it also.

Wolff cluster algorithm (PRL 62 (89), 361)

Principle: do the cluster decomposition as in S-W, but invert ('flip') only one randomly chosen cluster! In practice:

1. Choose random site i.
2. Study neighbouring sites j. If $s_j = s_i$, join site j to cluster with probability $p = 1 - \exp(-2\beta)$.
3. Repeat step 2 for site j, if it was joined to the cluster. Keep on doing this as long as the cluster grows.
4. When the cluster is finished, invert the spins which belong to it.

- Usually slightly more effective than S-W (the average size of the clusters is larger. Why?).
- The minimum cluster size = 1, maximum = volume.
- Nicely recursive.
- Satisfies detailed balance.

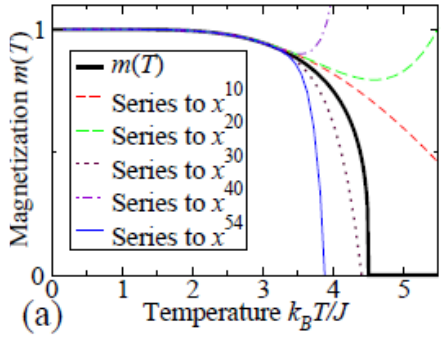


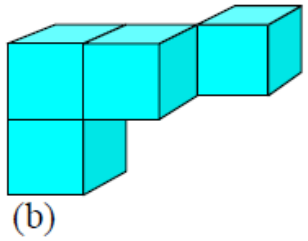
Autocorrelation function $C(t) \equiv \frac{\frac{1}{N-t}\sum_i O_i O_{i+t}}{\langle O^2 \rangle} \propto e^{-t/\tau}$

Order parameters & Ginzburg-Landau

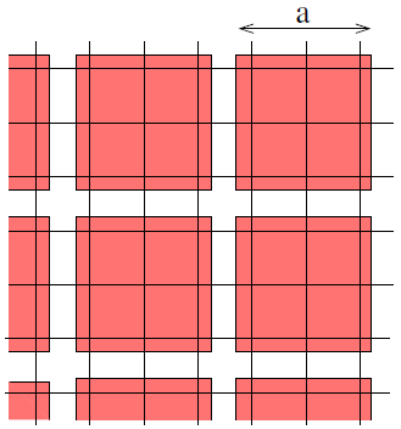
Inside a phase, an OP varies slowly but how do we detect the phase changes? (Example: magnetization for the Ising model in the FM phase).

GL: coarse-grain the system into patches of “large” size though smaller than the correlation length. Look, at what the FE looks like (and find the right normalization or partition function to get the FE right).





$$m(\mathbf{x}) = \frac{1}{N'} \sum_i s_i$$



What is GL theory?

Z sum over all configurations m, thus a *path integral*.

Conditions on the FE: locality (in m), symmetries (rotation, translation: original lattice), Z_2-symmetry (spin flips, we do now the Ising model), analyticity

Result (H breaks the parity symmetry, "-Hm") reads then:

$$Z = \int \mathcal{D}m(\mathbf{x})\ e^{-\beta F[m(\mathbf{x})]}$$

$$p[m(\mathbf{x})] = \frac{e^{-\beta F[m(\mathbf{x})]}}{Z}$$

$$F[m(\mathbf{x})] = \int d^d x\ \left[\frac{1}{2}\alpha_2(T)m^2 + \frac{1}{4}\alpha_4(T)m^4 + \frac{1}{2}\gamma(T)(\nabla m)^2 + \ldots\right]$$

See Chaikin and Lubensky

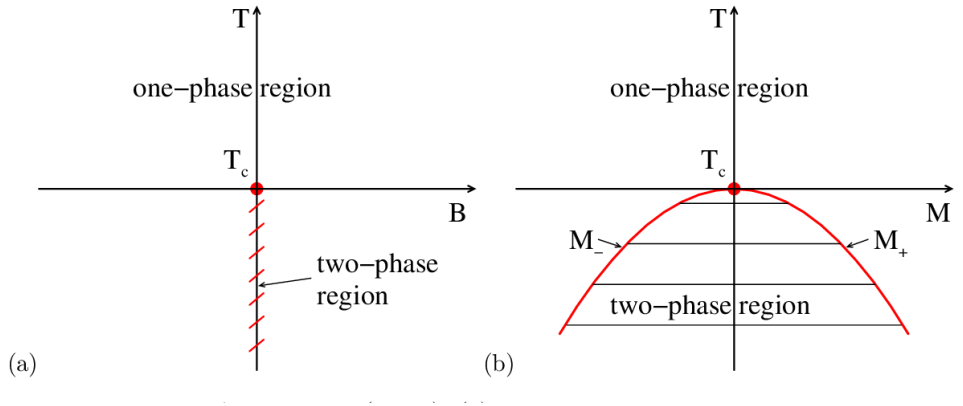
Consequences:

Mean-field solution (m constant): a 2nd order phase transition (continuous) related α_2 and the critical temperature. m(T,H) (B in the figure).

Similar arguments are used (applying the GL-theory) to superconductivity and to liquid crystals (nematic-isotropic transition, where different symmetry gives an extra α_3 term).

$$\alpha_2(T) \sim (T - T_c)$$

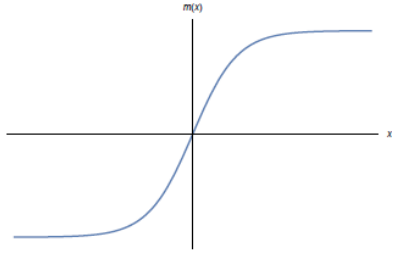
$$\alpha_4(T) \sim \frac{1}{3}T$$



Application of GL: domain wall

In the ordered phase go from one “domain” to another: Domain Wall. GL gives the energy and shape.

Applications: disorder, roughening… Lower critical dimension for order t to present!



$$\frac{\delta F}{\delta m(\mathbf{x})} = \alpha_2 m(\mathbf{x}) + \alpha_4 m^3(\mathbf{x}) - \gamma \nabla^2 m(\mathbf{x})$$

$$\left.\frac{\delta F}{\delta m}\right|_{m(\mathbf{x})} = 0 \quad \Rightarrow \quad \gamma \nabla^2 m = \alpha_2 m + \alpha_4 m^3$$

$$\gamma \frac{d^2 m}{dx^2} = \alpha_2 m + \alpha_4 m^3$$

$$m = m_0 \tanh\left(\frac{x - X}{W}\right) \qquad W = \sqrt{-\frac{2\gamma}{\alpha_2}}$$

$$F_{\text{wall}} \sim L^{d-1} \sqrt{-\frac{\gamma \alpha_2^3}{\alpha_4^2}}$$

What did we learn?

GL model: some “critical exponent” describing the behavior of quantities close to the critical temperature.

On general grounds, these are all not independent. Rescaling of time, space (correlation time, length), response to an external field is why.

How does one now compute the exponents? “Renormalization group” is the answer (K. Wilson, Nobel).

Homework

3.2 Damped oscillator (Sethna 10.3 p. 235) HOMEWORK (5 points)

Let us explore the fluctuating mass-on-a-spring. The coupling of the macroscopic motion to the internal degrees of freedom eventually damps any initial macroscopic oscillation; the remaining motions are microscopic thermal fluctuations. These fluctuations can be important, however, for nanomechanical and biological systems. In addition, the damped harmonic oscillator is a classic model for many atomic-scale physical processes, such as dielectric loss in insulators. Consider a damped, simple harmonic oscillator, forced with an external force f, obeying the equation of motion

$$\frac{\mathrm{d}^2\theta}{\mathrm{d}t^2} = -\omega_0^2\theta - \gamma\frac{\mathrm{d}\theta}{\mathrm{d}t} + \frac{f(t)}{m}. \tag{7}$$

(a) Susceptibility. Find the AC susceptibility $\tilde{\chi}(\omega)$ for the oscillator. Plot $\chi'(\omega)$ and $\chi''(\omega)$ for $\omega_0 = m = 1$ and $\gamma = 0.2, 2, 5$. (Hint: Fourier transform the equation of motion, and solve for $\tilde{\theta}$ in terms of $\tilde{f}$.)

(b) Causality and critical damping. Check, for positive damping γ, that your $\chi(\omega)$ is causal ($\chi(t) = 0$ for $t < 0$), by examining the singularities in the complex ω plane (Section 10.9 in Sethna). At what value of γ do the poles begin to sit on the imaginary axis? The system is overdamped, and the oscillations disappear, when the poles are on the imaginary axis.

(c) Dissipation and susceptibility. Given a forcing $f(t) = A\cos(\omega t)$, solve the equation and calculate $\theta(t)$. Calculate the average power dissipated by integrating your resulting formula for $f\mathrm{d}\theta/\mathrm{d}t$. Do your answers for the power and χ'' agree with the general formula for power dissipation, eqn 10.37 in Sethna ($p(\omega) = \frac{\omega|f_\omega|^2}{2}\chi''(\omega)$)?

(d) Correlations and thermal equilibrium. Use the fluctuation-dissipation theorem to calculate the correlation function $\tilde{C}(\omega)$ from $\chi''(\omega)$ ($\chi''(\omega) = \frac{\beta\omega}{2}\tilde{C}(\omega)$, see eqn 10.65 in Sethna p. 229), where

$$C(t - t') = \langle\theta(t)\theta(t')\rangle. \tag{8}$$

Find the equal-time correlation function $C(0) = \langle\theta^2\rangle$, and show that it satisfies the equipartition theorem. (Hints: Our oscillator is in a potential well $V(\theta) = \frac{1}{2}m\omega_0^2\theta^2$. Write $(\omega_0^2 - \omega^2)^2 + C^2\omega^2 = (\omega_0^2 - \omega^2 + iC\omega)(\omega_0^2 - \omega^2 - iC\omega)$ and do contour integration if you really, really like it. Or you can trust that the integral gives

$$\int_{-\infty}^{\infty}\mathrm{d}\omega\,\frac{1}{\omega}\chi''(\omega)e^{-i\omega t} \to \frac{\pi}{\omega_0^2 m}, \tag{9}$$

as $t \to 0$. Calculating these kinds of contour integrals is out of the scope of this course.)

Take home

- Take home (Sethna Chapter 10 plus additional material Ginzburg-Landau theory: Chaikin-Lubensky, Principles of Condensed Matter Physics, Ch. 4.1-4.4 and Ch. 10.1 and 10.2.).

  Read the chapter, and the parts of Ginzburg-Landau theory. Check also the cluster Monte Carlo algorithms (the web is full of lecture notes, and Wikipedia has a good article on the S-W algorithm): do you think you understand why they work?

  Here we introduce the Ising model as the paradigm of statistical physics and phase transitions. The book discusses the model and how to study it by computational means. The CL-part tells how a "coarse-grained" theory is formed for the Ising model (and its variants and other systems; "phase-field model" is a key concept).

  The random field Ising model (RFIM) comes when you introduce the random fields to each site. The RFIM has a phase diagram like the normal Ising except that random fields can destroy ferromagnetic order at any temperature if they are strong enough.

  How would the random field affect a) a GL-theory (what is the free energy like?) and b) the physics of a domain wall?

  Then check the following application of the model: https://link.springer.com/article/10.1140/epjb/e2005-00307-0

  Read through the paper. How would you simulate the model - how do the random fields enter the picture? Put the model on a 2D lattice, with a fixed set of neighbors for each "opinion" for that purpose.
  What kind of transitions would you expect in this system?

  (For those interested please see https://www.cfm.fr/work-with-us/#Our%20internships for summer jobs)