

Advanced Statistical Physics

Part II : Phase Transitions and Critical Phenomena

Zakaria Mzaouali

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Mohammed V University.
Rabat, Morocco.

1. C.Ngo, H.Ngo - Physique Statistique - Chapter 10 & 11.
2. Nigel Goldenfeld - Lectures On Phase Transitions And The Renormalization Group - Chapter 2, 3 & 5.

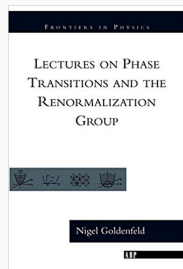
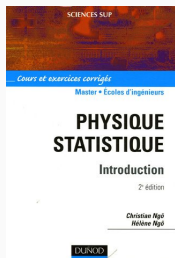


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Introduction

What is a Phase ? What is a phase transition ?

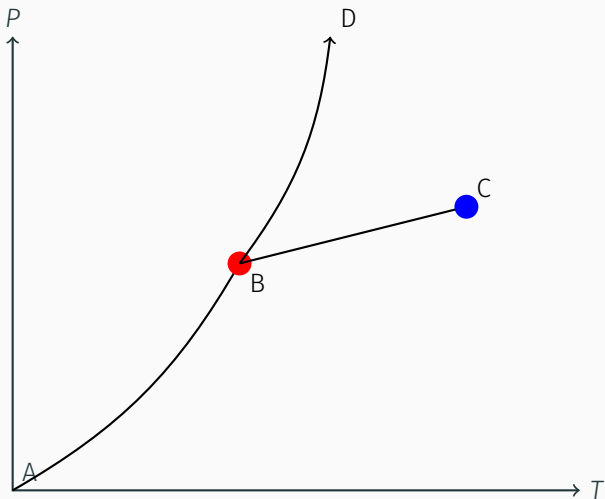


Figure 1: Phase diagram of water.

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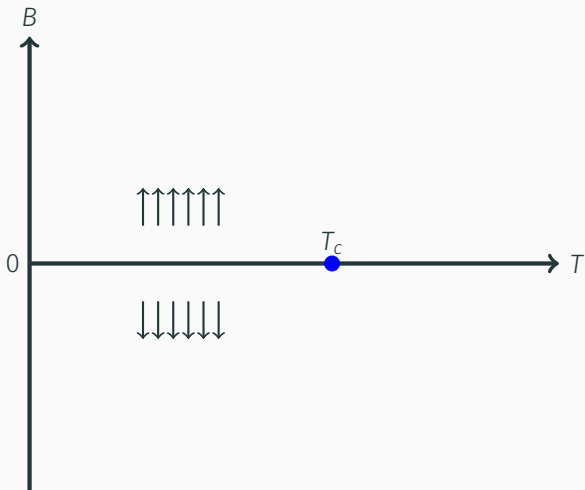
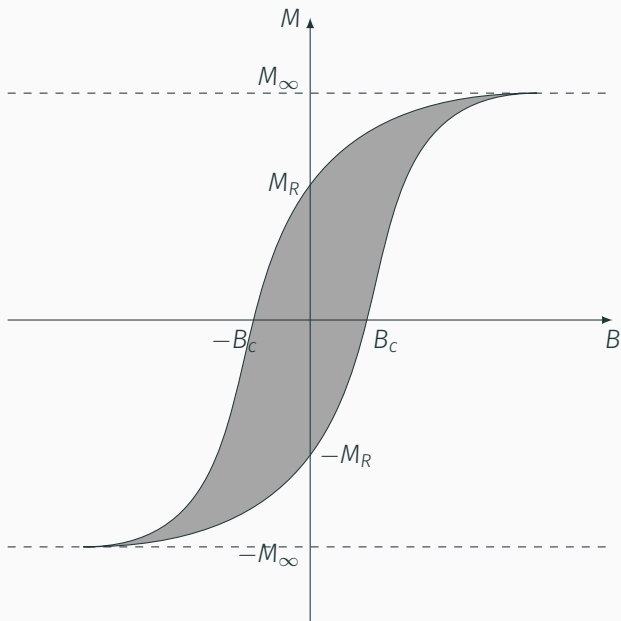


Figure 2: Phase diagram of a ferromagnetic material.

What is a Phase ? What is a phase transition ?



How Phase Transitions Occur in Principle

Preliminaries : Convexity

$f(x)$ is a concave function of x if :

$$f\left(\frac{x_1 + x_2}{2}\right) \leq \frac{f(x_1) + f(x_2)}{2} \quad \text{for all } x_1 \text{ and } x_2.$$

Which means that the chord joining the points $f(x_1)$ and $f(x_2)$ lies above of $f(x)$ for all x in $x_1 < x < x_2$.

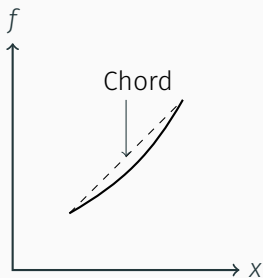


Figure 3: Convex function.

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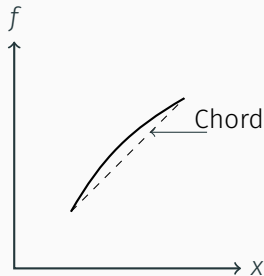


Figure 4: Concave function

Consequences of the convexity and the concavity

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Consequences of the convexity and the concavity

The specific heat and the susceptibility (for magnetic materials) are positive thermodynamical response function, which implies that the free energy F is convex. This is a direct consequence of Le Chatelier's principle for stable equilibrium which states that : if a system is in thermal equilibrium any small spontaneous fluctuation in the system parameter, the system gives rise to certain processes that tends to restore the system back to equilibrium.

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The existence of the thermodynamic limit is not trivial as it fails to exist for some systems.

Preliminaries : Existence of the Thermodynamic limit

Consider a charged system at $T = 0$ in 3 dimensions, the interaction between two particles separated by a distance r is given by Coulomb's law :

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$$\begin{aligned} E &= \int_0^R \left(\frac{4}{3}\pi r^3 \rho \right) \frac{A}{r} 4\pi r^2 \rho dr \\ &= A \frac{(4\pi)^2}{15} \rho^2 R^5. \end{aligned}$$

The energy per unit volume is then : $\epsilon = A \frac{(4\pi)^2}{15} \rho^2 R^2$, which diverges as $R \rightarrow \infty$.

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Inverse square law forces like gravity and electrostatics are too long-ranged to permit thermodynamic behaviour

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Taking the limit $R \rightarrow \infty$, the system is stable only when $m > d$. The thermodynamic limit exist then only when $m > d$.

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Then, a phase is just a region of analyticity of $f_b[K]$ and loci of co-dimension $C = D - D_s = 1$ is called a phase boundary.

$f_b[K]$ can be used also to classify phase transitions :

- **First order phase transitions**

If one or more $\partial f_b / \partial K_i$ are discontinuous across a phase boundary, the transition is first order.

- **Continuous phase transitions**

If the first derivative of $f_b[K]$ is continuous across the phase boundary, the transition is said to be continuous phase transitions (or a second order phase transition)

The role model

The Ising model

The Ising model can be written as :

$$-H_{\Omega} = \sum_{i \in \Omega} H_i S_i + \sum_{ij} J_{ij} S_i S_j + \sum_{ijk} K_{ijk} S_i S_j S_k + \dots \quad (1)$$

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The free energy is given by : $F_{\Omega}(T, H_i, J_{ij}) = -k_b T \log \text{Tr} e^{-\beta H_{\Omega}}$.

The thermodynamical properties can be calculated through F_{Ω} , for example the magnetization at site i is :

$$\frac{\partial F_{\Omega}}{\partial H_i} = -k_B T \frac{1}{\text{Tr} e^{-\beta H_{\Omega}}} \text{Tr} \frac{S_i}{k_b T} e^{-\beta H_{\Omega}} = -\langle S_i \rangle_{\Omega}$$

The Ising model : Spin-reversal symmetry

The Ising model is Z_2 symmetric. That is a rotation of π of all the spins, leave the system energy unchanged. Mathematically, this implies that :

$$H_{\Omega}(H, J, S_i) = H_{\Omega}(-H, J, -S_i).$$

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Thus :

$$\begin{aligned} Z_{\Omega}(-H, J, T) &= \sum_{S_i=\pm 1} e^{-\beta H_{\Omega}(-H, J, S_i)} \\ &= \sum_{S_i=\pm 1} e^{-\beta H_{\Omega}(-H, J, -S_i)} \\ &= \sum_{S_i=\pm 1} e^{-\beta H_{\Omega}(H, J, S_i)} \\ &= Z_{\Omega}(H, J, T). \end{aligned}$$

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The free energy is then :

$$F(H, J, T) = F(-H, J, T)$$

The Ising model : Sub-lattice symmetry

This symmetry emerges at zero magnetic field ($H = 0$). We divide the lattice into two interpenetrating lattices A and B . The spins of lattice A interacts only with the ones in the lattice B

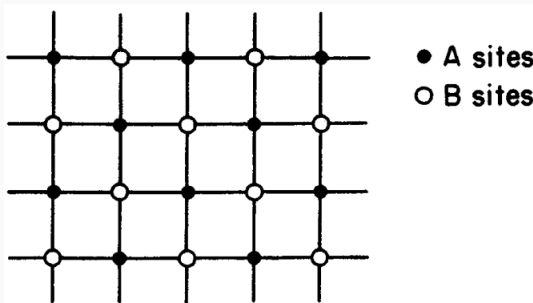


Figure 5: Two interpenetrating lattices A and B

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The Hamiltonian is $H_{\Omega}(0, J, S_i^A, S_i^B) = -J \sum_{\langle ij \rangle} S_i^A S_j^B$.

The sub-lattice symmetry implies that :

$$H_{\Omega}(0, -J, S_i^A, S_i^B) = H_{\Omega}(0, J, -S_i^A, S_i^B) = H_{\Omega}(0, J, S_i^A, -S_i^B).$$

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In zero field we write the partition function :

$$\begin{aligned} Z_{\Omega}(0, -J, T) &= \text{Tr} e^{-\beta H_{\Omega}(0, -J, T)} \\ &= \sum_{S_i^A} \sum_{S_j^B} e^{-\beta H_{\Omega}(0, -J, S_i^A, S_j^B)} \\ &= \sum_{S_i^A} \sum_{S_j^B} e^{-\beta H_{\Omega}(0, J, -S_i^A, S_j^B)} \\ &= \sum_{S_i^A} \sum_{S_j^B} e^{-\beta H_{\Omega}(0, J, S_i^A, S_j^B)} \\ &= Z_{\Omega}(0, J, T). \end{aligned}$$

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The sub-lattice symmetry implies that the thermodynamics of the ferromagnetic Ising model and that of the anti-ferromagnetic Ising model are the same at zero magnetic field.

The Ising model : Existence of Phase Transitions

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The phase diagram is a guide map of the different phases a system or a model has. How do we build such a map ? One strategy to construct the phase diagram is through *the energy-entropy argument*. We study the free energy at high and low temperatures and if the macroscopic states of the system obtained by the two limits are different, then we conclude that at least one phase transition has occurred at some temperature.

The Ising model : 0T Phase diagram

Consider the Ising model in d -dimensions at $T = 0$, then $F=E$.

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Suppose that we have available the energy configurations of our system.

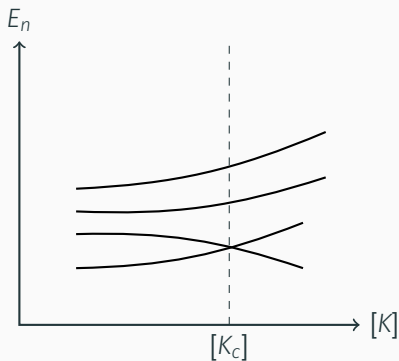


Figure 6: The mechanism of level crossing

The Ising model : 0T Phase diagram

The ground state is obtained for $J > 0$ by noticing that $-J \sum_{\langle ij \rangle} S_i S_j$ is minimized when $S_i = S_j$ and the term $-H \sum_i S_i$ is minimized by $S_i = +1$ when $H > 0$ and $S_i = -1$ when $H < 0$.

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$$S_i = \begin{cases} +1 & H > 0, J > 0; \\ -1 & H < 0, J > 0. \end{cases}$$

The magnetization is then :

$$M_\Omega = \frac{1}{N(\Omega)} \sum_{i \in \Omega} S_i = \begin{cases} +1 & H > 0; \\ -1 & H < 0. \end{cases}$$

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A phase transition occurs at zero temperature and at zero magnetic field.

The Ising model : 1D phase diagram

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$$\Delta F = \Delta E - T\Delta S = 2J - k_b T \ln N.$$

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There is no long range order. Thus, the 1D Ising model has no phase transitions at $H = 0$

The Ising model : 2D phase diagram

We consider again a domain of flipped spins, in a background of spins with long range order, but this time the domain is two dimensional. What is the energy difference ? and what is the entropy?

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The internal energy change of a domain of length L is $\Delta E = 2JL$. The entropy can be estimated by enumerating the different possibilities of the domain wall, it turns out that this number is proportional to the coordinate number of the lattice z . The entropy is then $\Delta S = k_b L \log(z - 1)$ and the free energy is:

$$\Delta F = 2JL - (\log(z - 1)) k_b TL.$$

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We can speak of phase transitions at finite temperatures only in the 2D Ising model or above

The impossibility theorem

The impossibility of phase transitions can be seen immediately from the spin-reversal symmetry of the Ising model. We know that the free energy satisfies the following :

$$F_{\Omega}(H, J, T) = F_{\Omega}(-H, J, T),$$

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$$N(\Omega)M_{\Omega}(H) = -\frac{\partial F_{\Omega}(H)}{\partial H} = -\frac{\partial F_{\Omega}(-H)}{\partial H} = \frac{\partial F_{\Omega}(-H)}{\partial -H} = -N(\Omega)M_{\Omega}(-H).$$

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This is the **impossibility theorem** it shows that the magnetization in $H = 0$ should be zero, a result that contradicts our previous finding.

What has gone wrong ?

Spontaneous Symmetry Breaking

When $N \rightarrow \infty$ the free energy develops a discontinuity in its first derivative, and knowing the fact that $F(H)$ is a convex function, the condition $F(H) = F(-H)$ does not *imply* $M(0) = 0$, for that to happen we need to add the assumption of the smoothness of the free energy at $H = 0$ and that the left and right derivatives are equal.

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$$F(H) = F(0) + O(H^p) \quad p > 1$$

and

$$\lim_{\epsilon \rightarrow 0} \frac{F(+\epsilon) - F(0)}{\epsilon} = \lim_{\epsilon \rightarrow 0} \frac{F(-\epsilon) - F(0)}{\epsilon} = 0$$

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We can then turn around the impossibility theorem and still satisfy the analytical properties of the free energy by writing :

$$F(H) = F(0) - M_s |H| + O(H^p) \quad p > 1$$

which is not differentiable at $H = 0$, but still hold the convexity property as depicted Fig. 7

Spontaneous Symmetry Breaking

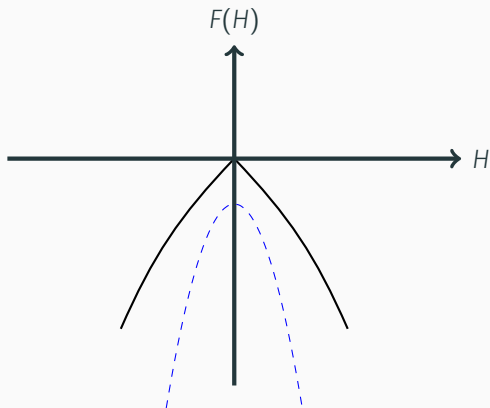


Figure 7: The free energy as function of H for a finite system (dashed line) and for an infinite system (solid line)

Spontaneous Symmetry Breaking

$$\frac{\partial F}{\partial H} = \begin{cases} -M_s + O(H^{p-1}), & H > 0 \\ -M_s + O(H^{p-1}), & H < 0. \end{cases}$$

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As $|H| \rightarrow 0$, we have :

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are not equal. Even though the Hamiltonian is invariant under spin reversal, the expectation values do not follow this symmetry, so that

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How Phase Transitions Occur in Practice

Transfer Matrix

We start with the 1D nearest-neighbors Ising model.

$$-H_{\Omega} = H \sum_{i \in \Omega} S_i + \sum_{\langle ij \rangle} J_{ij} S_i S_j, \quad J > 0.$$

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$$\begin{aligned} Z_N(h, K) &= \text{Tr} \exp \left[h \sum_i S_i + K \sum_i S_i S_{i+1} \right] \\ &= \sum_{S_1} \dots \sum_{S_N} \left[e^{\frac{h}{2}(S_1+S_2)+KS_1S_2} \right] \cdot \left[e^{\frac{h}{2}(S_2+S_3)+KS_2S_3} \right] \dots \left[e^{\frac{h}{2}(S_N+S_1)+KS_NS_1} \right]. \end{aligned}$$

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Each term in the partition function can be written as a matrix T :

$$T_{S_1 S_2} = e^{\frac{h}{2}(S_1+S_2)+KS_1S_2},$$

whose elements are :

$$T = \begin{pmatrix} T_{1,1} & T_{1,-1} \\ T_{-1,1} & T_{-1,-1} \end{pmatrix} = \begin{pmatrix} e^{h+K} & e^{-K} \\ e^{-K} & e^{-h+K} \end{pmatrix}, \quad (3)$$

Transfer Matrix

the partition function can be re-written in terms of the matrix T as :

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Thus :

$$Z_N(h, K) = \text{Tr} (T^N),$$

since T is real and symmetric, we diagonalize it by writing :

$$T' = S^{-1}TS,$$

where S is a matrix whose rows and columns are eigenvectors of T .

Then :

$$T' = \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix},$$

where λ_1 and λ_2 are the eigenvalues of T . The cyclic property of the trace operation implies that $\text{Tr} (T') = \text{Tr} (T)$, so that :

$$\text{Tr} (T^N) = \lambda_1^N + \lambda_2^N.$$

Transfer Matrix

Assuming that $\lambda_1 > \lambda_2$, we have :

$$Z_N(h, K) = \lambda_1^N \left(1 + \left[\frac{\lambda_2}{\lambda_1} \right]^N \right),$$

and taking the thermodynamic limit $N \rightarrow \infty$, we get :

$$Z_N(h, K) \approx \lambda_1^N (1 + O(e^{-\alpha N})),$$

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Solving Eq. 3, we obtain : $\lambda_{1,2} = e^K \left[\cosh h \pm \sqrt{\sinh^2 h + e^{-4K}} \right]$.

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The free energy of the one dimensional Ising model in an external magnetic field is :

$$\frac{F_N(h, K, T)}{N} = -J - k_B T \log \left[\cosh h + \sqrt{\sinh^2 h + e^{-4K}} \right] \quad (4)$$

Perron's Theorem

Theorem

For an $N \times N$ matrix ($N < \infty$) A , with positive entries A_{ij} for all (i, j) , the largest eigenvalue satisfies the following :

- 1. real and positive*
- 2. non-degenerate*
- 3. an analytic function of A_{ij}*

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Inspecting Eq. 4 leads to the conclusion that to have non-zero temperature phase transitions, λ_1 should be either non-analytic, degenerate ($\lambda_1 = \lambda_2$), or $\lambda_1 = 0$. On the other side, the transfer matrix for 1D systems with sufficiently short-ranged interactions satisfy the Perron's theorem, that is $\lambda_1 \neq 0$, $\lambda_1 \neq \lambda_2$ and λ_1 in analytic.

Thus, we immediately conclude that there are no finite temperature phase transitions in the 1D Ising model.

Transfer Matrix : 0T Ising model

At $T = 0$ ($K \rightarrow \infty$): $\lambda_1 = e^K \left[\cosh h + \sqrt{\sinh^2 h (1 + O(e^{-4K}))} \right] = e^{K+|h|}$.

Then, the free energy and the magnetization are given by :

$$F = -Nk_B T (K + |h|) + O(T^2) = -N(J + |H|), \quad M = -\frac{1}{N} \frac{\partial F}{\partial H} = \begin{cases} 1 & H > 0; \\ -1 & H < 0, \end{cases}$$

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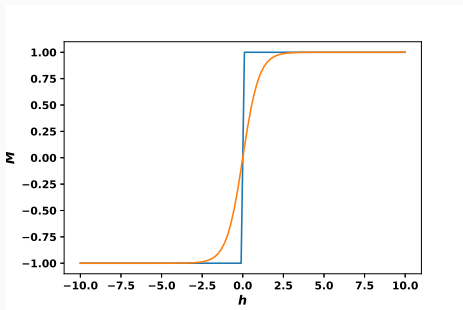


Figure 8: Magnetization vs the magnetic field. Blue line correspond to $T = 0$, while the orange line is for a non-zero temperature.

We switch off the magnetic field to calculate the specific heat C_V and the magnetic susceptibility χ_T .

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The partition function is $Z = (2 \cosh K)^N$ as $N \rightarrow \infty$ and the free energy is : $F = -k_B T N [K + \log (1 + e^{-2K})]$, with limits :

$$F/N = \begin{cases} -J & T \rightarrow 0 (K \rightarrow \infty); \\ -k_B T \log 2 & T \rightarrow \infty (K \rightarrow 0). \end{cases}$$

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$$C_V = \frac{\partial E}{\partial T} = -\frac{1}{k_B T^2} \frac{\partial E}{\partial \beta} = \frac{1}{k_B T^2} \frac{\partial^2 Z}{\partial \beta^2} = \frac{NJ^2}{k_B T^2} \operatorname{sech}^2 \left(\frac{J}{k_B T} \right).$$

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The heat capacity does not show any singularity, however it exhibit a peak at $J \sim k_B T$, a phenomena known as **Schottky anomaly**

The magnetic susceptibility is : $\chi = \frac{\partial M}{\partial H} = \beta \frac{\partial M}{\partial h} = \beta \frac{\partial}{\partial h} \left(\frac{\sinh h}{\sqrt{\sinh^2 h + e^{-4K}}} \right)$

Thermodynamics

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for small field ($h \rightarrow 0$), it reduces to:

$$\chi \sim \begin{cases} \frac{1}{k_b T}, & T \rightarrow \infty (\text{Curie's law}); \\ \frac{e^{\frac{2J}{k_B T}}}{k_b T}, & T \rightarrow 0 \end{cases}$$

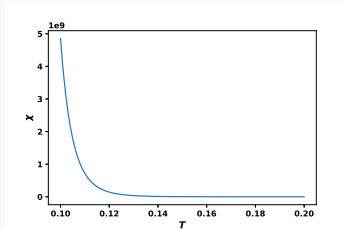


Figure 9: Magnetic susceptibility vs temperature at zero magnetic field.

Correlation functions

In statistical mechanics, a correlation function is a measure of order in a system, more concretely they describe how microscopic variables, such as spin and density, co-vary with one another across space and time.

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The two point correlation function is defined as :

$$G(i, j) = \langle S_i S_j \rangle - \langle S_i \rangle \langle S_j \rangle = \langle S_i S_j \rangle, \quad (\text{For } T > 0 \text{ and } h = 0 : \langle S_i \rangle = \langle S_j \rangle = 0).$$

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Then :

$$\langle S_i S_{i+1} \rangle = \frac{1}{Z} \sum_{\{S\}} S_i S_{i+1} e^{KS_i S_{i+1}} = \frac{\partial \log Z}{\partial K}.$$

Correlation functions

The partition function $Z_{i,i+1}$ is :

$$Z = \sum_{S_i = \pm 1} e^{KS_i S_{i+1}} = 2 (e^K + e^{-K}) = 2^2 \cosh(K).$$

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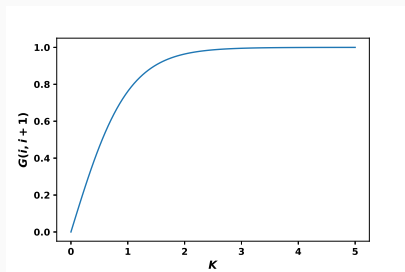


Figure 10: Nearest neighbours correlation function vs temperature. For high temperatures ($K \rightarrow 0$) the two spins are less correlated, while for low temperatures ($K \rightarrow \infty$) the spins are highly correlated

Correlation functions

It is straightforward to generalize the result beyond $(i, i + 1)$:

$$\begin{aligned}G(i, i + j) &= \langle S_i S_{i+j} \rangle \\ &= \tanh(K_i) \tanh(K_{i+1}) \dots \tanh(K_{i+j-1}) \\ &= (\tanh(K))^j ,\end{aligned}$$

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where $\xi = \frac{1}{\log(\coth K)}$ is called : **the correlation length**

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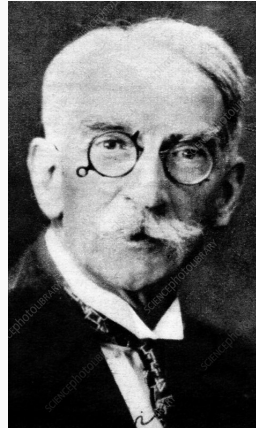
$$\xi^{-1} = \log\left(\frac{\lambda_1}{\lambda_2}\right). \quad (5)$$

A clear indication of a phase transition is a divergence in the correlation length, for that to happen we need $\lambda_1 = \lambda_2$ (the largest eigenvalue need to be degenerate). This is a general result.

Weiss' Mean Field Theory

Mean field theory :

1. Goal ? : treating interacting statistical mechanical systems
2. Idea ? : for a system of N particles, we replace the interaction between the particles by a mean potential and we forget about fluctuations.
3. Effectiveness ? : when the fluctuation are weak, which not the case around the critical region



Weiss' Mean Field Theory

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In this approach, the Ising model can be written as : $H_{\Omega} = -\sum_i S_i H_i$,
where

$$H_i = \underbrace{H}_{\text{magnetic field}} + \underbrace{\sum_j J_{ij} \langle S_j \rangle}_{\text{the mean field}} + \underbrace{\sum_j J_{ij} (S_j - \langle S_j \rangle)}_{\text{the fluctuations}}.$$

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$$H_i = \underbrace{H}_{\text{magnetic field}} + \underbrace{\sum_j J_{ij} \langle S_j \rangle}_{\text{the mean field}} + \underbrace{\sum_j J_{ij} (S_j - \langle S_j \rangle)}_{\text{the fluctuations}}.$$

for a d -dimensional hypercubic lattice we have : $H_i = H + 2dJm$,

Weiss' Mean Field Theory: Critical exponents

Then, the magnetization is :

$$M = \tanh \left(\frac{H + 2dJm}{k_B T} \right),$$

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$$M = \tanh\left(\frac{H}{k_B T} + m\tau\right) = \frac{\tanh\left(\frac{H}{k_B T}\right) + \tanh m\tau}{1 + \tanh\left(\frac{H}{k_B T}\right) \tanh m\tau},$$

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for weak H and small m , we can expand Eq. 6 as :

$$\frac{H}{k_B T} \approx M(1 - \tau) + M^3 \left(\tau - \tau^2 + \frac{\tau^3}{3} + \dots \right) + \dots \quad (7)$$

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For zero magnetic field and when $T \rightarrow T_c^-$, we have :

$$M^2 \approx 3 \frac{T_c - T}{T} + \dots$$

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The critical isotherm is the curve in the H - M plan corresponding to $T = T_c$. Near the critical point, it is described by a critical exponent δ :

$$H \sim M^\delta.$$

Setting $\tau = 1$ in Eq. 7, we find $\delta = 3$. That is :

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The isothermal magnetic susceptibility also diverges near T_c :

$$\chi_T = \frac{\partial M}{\partial H},$$

from Eq. 7, we get :

$$\frac{1}{k_B T} = \chi_T(1 - \tau) + 3M^2\chi_T(\tau - \tau^2 + \frac{1}{3}\tau^3).$$

Weiss' Mean Field Theory: Critical exponents

$M = 0$ for $T > T_c$, then :

$$\chi_T = \frac{1}{k_B} \frac{1}{T - T_c} + \dots \quad (8)$$

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$$M = \sqrt{3} \left(\frac{T_c - T}{T} \right)^{1/2} + \dots$$

which yields to :

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The critical exponent α of the specific heat is calculated from the free energy written in the MFA approximation as :

$$F_m = -k_B T \ln [2 \cosh (\beta J 2 d m)],$$

Weiss' Mean Field Theory : Critical exponents

Note that $\cosh(x) = 1 + \frac{x^2}{2!} + \frac{x^4}{4!} + \dots$ and that $M = 0$ for $T > T_c$ while $M = \left(3\frac{T_c - T}{T}\right)^{1/2}$ for $T < T_c$.

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$$C = \begin{cases} \frac{3}{2}k_B N & T < T_c \\ 0 & T > T_c. \end{cases}$$

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In summary, we have derived the following critical exponents :

$$\beta = 1/2, \delta = 3, \gamma = 1 \text{ and } \alpha = 0.$$

Weiss' Mean Field Theory : Critical exponents

Now, we derive an important relationship between the isothermal magnetic susceptibility and the correlations functions.

$$Z = \text{Tr} \exp \left[H\beta \sum_i S_i + \beta J \sum_{\langle ij \rangle} S_i S_j \right],$$

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On the other side :

$$\begin{aligned} \chi_T &= \frac{\partial M}{\partial H} = \frac{1}{\beta N} \frac{\partial^2 \log Z}{\partial H^2} = \frac{1}{N} k_B T \left[\frac{1}{Z} \frac{\partial^2 Z}{\partial H^2} - \frac{1}{Z^2} \left(\frac{\partial Z}{\partial H} \right)^2 \right] \\ &= \frac{1}{N} (k_B T)^{-1} \left[\sum_{ij} \langle S_i S_j \rangle - \left(\sum_i \langle S_i \rangle \right)^2 \right] = \frac{1}{N} (k_B T)^{-1} \sum_{ij} G(r_i - r_j) \\ &= (k_B T)^{-1} \sum_i G(x_i) = (a^d k_B T)^{-1} \int_{\Omega} d^d r G(r). \end{aligned}$$

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with $z = r/\xi$. Thus :

$$\xi \sim \left(\frac{T_c - T}{T}\right)^{-\nu}, \quad (10)$$

with $\nu = 1/2$.

Weiss' Mean Field Theory : Critical exponents

The last critical exponent we mention is η , which describe how the point correlation function behave at long distances at the critical point. $G(r)$ for long distances near the critical point is given by : $G(r) \sim r^{-(d-2+\eta)}$, with $\eta = 0$. In principal η can be non zero.

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Exponent	Mean Field	Experiment	2D Ising	3D Ising
α	0	0.110-0.116	0	0.110
β	1/2	0.316-0.327	1/8	0.325 ± 0.0015
γ	1	1.23-1.25	7/4	1.2405 ± 0.0015
δ	3	4.6-4.9	15	4.82
ν	1/2	0.625 ± 0.010	1	0.630
η	0	0.016 - 0.06	1/4	0.032 ± 0.003

Table 1: Critical exponents for the Ising universality class

Can we trust MFT ?

From Tab. 1, there is a clear discrepancy between the critical exponents obtained by the mean field approximation and the experimental result while the exponents of the 3D Ising model are in accordance with experience.

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The mean field approximation is clearly not a good choice for magnetic systems.

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The critical exponents satisfy the scaling relations obtained by thermodynamic considerations, they are given by :

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The precision of the mean field approximation increases as we increase the dimension of the system. In fact, from the scaling relation $2 - \alpha = d\nu$, where d is the dimension of the system, we can deduce the critical dimension at which we get precise results from the mean field approximation. Since $\alpha = 0$ and $\nu = 1/2$, d_c must be 4.

Landau Theory of Phase Transitions.

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Landau Theory of Phase Transitions :

1. A theory for all phase transitions.
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3. Procedure ? : Writing the potential as function of the order parameter m . The minimas with respect to m should describe the thermodynamic properties of the system at the critical point.



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Landau Theory

This theory consists of writing a function L called *Landau free energy* or *Landau functional* in terms of the order parameter η and the coupling constants $\{K_i\}$, where we keep only the terms compatible with the symmetries of the system.

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$$L = \sum_{n=0}^{\infty} a_n([K])\eta^n.$$

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3. $\eta=0$ in the disordered phase, while it is small and non zero in the ordered phase near T_c . Thus, for $T > T_c$ we solve the minimum equation for L by $\eta = 0$ and for $T < T_c$ $\eta \neq 0$ solves the minimum equation. For a homogeneous system we can write :

$$L = \sum_{n=0}^4 a_n([K])\eta^n. \quad (11)$$

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$$\frac{\partial L}{\partial \eta} = a_1 + 2a_2\eta + 3a_3\eta^2 + 4a_4\eta^3 = 0. \quad (12)$$

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$a_0([K], T)$ represents the value L in the disordered phase ($\eta = 0$ for $T > T_c$), it describes the degrees of freedom of the system that cannot be understood via the order parameter

For a_2 and a_4 expanding in temperature near T_c , we obtain :

$$a_4 = a_4^0 + (T - T_c) a_4^1 + \dots$$

$$a_2 = a_2^0 + \frac{(T - T_c)}{T_c} a_2^1 + O\left((T - T_c)^2\right),$$

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Since $\partial^2 L / \partial \eta^2 = 1/\chi = 0$ as $T \rightarrow T_c$, one has $a_2^0 = 0$ and :

$$a_2 = \frac{(T - T_c)}{T_c} a_2^1 + O\left((T - T_c)^2\right).$$

The extension to the case $H \neq 0$ for the Ising ferromagnet is immediate

$$L = a \left(\frac{T - T_c}{T_c} \right) \eta^2 + \frac{1}{2} b \eta^4 - H \eta. \quad (14)$$

Landau Theory : Continuous Phase Transitions

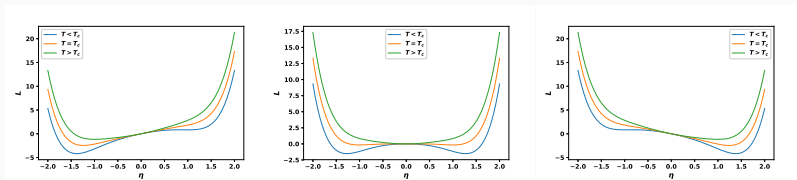


Figure 11: Landau free energy for different values of T and H . From left to right : $H < 0$, $H = 0$ and $H > 0$.

Landau Theory : Continuous Phase Transitions

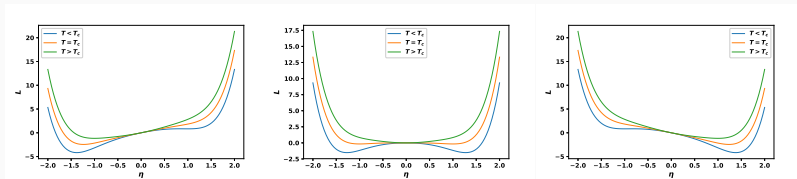


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When $H = 0$ and for $T > T_c$, L has a minimum at $\eta = 0$. When $T = T_c$ Landau potential has zero curvature at $\eta = 0$ while $\eta = 0$ is still the global minimum. For $T < T_c$, Landau free energy shows two degenerate minima at $\eta = \pm n_s(T)$

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Solving $\partial L / \partial \eta = 0$ for η we can read off the critical exponent β . We have :

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The critical exponent α of the heat capacity can be extracted by writing : $C_V = -T\partial^2 L/\partial T^2$, then :

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which shows that the heat capacity exhibit a discontinuity and that

$$\alpha = 0$$

For the case $H > 0$. Taking the derivative with respect to H in Eq. 14 gives :

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On the critical isotherm, that is on $t = 0$. We have $H \propto \eta^3$ and we read the critical exponent $\delta = 3$.

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On the critical isotherm, that is on $t = 0$. We have $H \propto \eta^3$ and we read the critical exponent $\delta = 3$. The isothermal susceptibility χ_T can be computed by taking the derivative of Eq. 15 with respect to H . That is :

$$\chi_T = \frac{\partial\eta(H)}{\partial H} = \frac{1}{2(at + 3b\eta(H)^2)}, \quad (16)$$

Landau Theory : Continuous Phase Transitions

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where $\eta(H)$ is a solution of Eq. 15. For $t > 0$, we have $\eta = 0$, then $\chi_T \propto t^{-1}$ while for $t < 0$, we have $\eta = (-at/b)^{1/2}$ and $\chi_T \propto t^{-1}$. Thus, the critical exponent is $\gamma = 1$.

What happens if we add a cubic term in L ?

Landau Theory : First order Phase Transitions

What happens if we add a cubic term in L ? In general we have :

$$L = aT\eta^2 + \frac{1}{2}b\eta^4 + C\eta^3 - H\eta. \quad (17)$$

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The solution $\eta \neq 0$ is real when the argument of the square root is positive, i.e. $\sqrt{c^2 - at/b} > 0$. That is, $t < t^* = bc^2/a$

Landau Theory : First order Phase Transitions

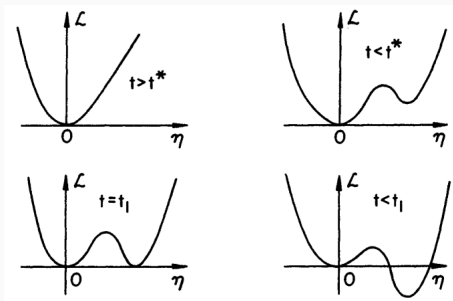


Figure 12: L as a function of η for different values of T showing how Landau's theory describes first order phase transitions

Landau Theory : First order Phase Transitions

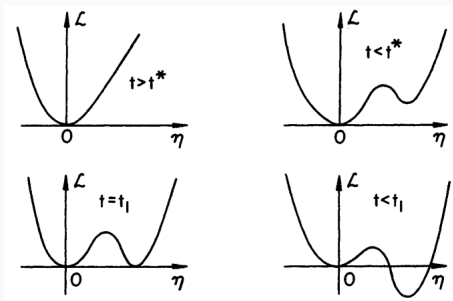


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A sufficient but not necessary condition of the occurrence of continuous phase transitions is that there are no cubic terms in the potential. In general, the cubic term causes a first order phase transition.

Thank you for your attendance
and your attention.