

RANDOMLY DILUTED MODELS

Ferromagnets and antiferromagnets are systems which show a high-temperature paramagnetic phase and a low-temperature ferromagnetic phase.

They are characterized by considering the behavior of the **MAGNETIZATION**. If the material is placed in an external magnetic field H and the temperature is sufficiently low, the system shows a spontaneous magnetization.

In practice: for $|H| \rightarrow 0$

$$\begin{aligned} M &\rightarrow 0 && \text{for } T > T_c, \\ M &\rightarrow M_0(T) && \text{for } T < T_c, \end{aligned}$$

T_c is called **Curie** temperature.

NOTE: the magnetization cannot be measured directly in experiments. Usually, one measures some indirect effect which is related to the presence of the magnetization. For instance, to verify the 2D Ising behavior in thin films, one can send ions on the film and measure the polarization of the reflected beam: $P \propto M$, so that $P \neq 0$ below T_c and $P = 0$ above T_c .

Close to T_c some features are **UNIVERSAL**, i.e. they do not depend on the specific material one is considering, but only on some general properties:

1. space dimension,
2. symmetry of the Hamiltonian,
3. symmetry of the ground state,
4. range of the interactions.

Moreover, the presence of disorder may change the critical behavior.

Critical exponents are a **UNIVERSAL** feature of continuous transitions. For instance, one defines an exponent β from the behavior of the magnetization for $T \rightarrow T_c$, $T < T_c$:

$$M(T) = (T_c - T)^\beta$$

Other scaling relations:

$$\begin{aligned}\chi &= |T - T_c|^{-\gamma} \\ \xi &= |T - T_c|^{-\nu}\end{aligned}$$

Here χ is the magnetic susceptibility defined by

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

while ξ measures the spatial correlations and can be measured in scattering experiments. If the system is ferromagnetic and $S(\mathbf{q})$ is the structure factor normalized so that $S(0) = 1$, then for $\mathbf{q} \rightarrow 0$,

$$S(\mathbf{q}) = 1 - q^2 \xi^2 + O(q^4).$$

The exponents β , γ , and ν are **UNIVERSAL**.

(Anti)-ferromagnetic materials are usually modeled by considering:

1. Heisenberg spins \mathbf{S}_i , where i labels a lattice site;
2. a Hamiltonian given by

$$H = - \sum_{ij} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j + D_{\text{Is}} \sum_i S_{z,i}^2 + D_{\text{cubic}} \sum_i S_{z,i}^4 + \dots$$

OBSERVATIONS:

1. The Heisenberg spins are quantum objects. However, since the Curie transition is a finite-temperature transition, quantum effects are irrelevant. Roughly: the spacing among the quantum levels is much smaller than the thermal energy $k_B T_c$. Thus, we can disregard the energy quantization and take the classical limit. Thus, in order to determine universal properties (and only for that) we can assume \mathbf{S}_i to be a unit three-component vector.

2. The first term is the exchange interaction, which is a pure quantum effect (it is a consequence of the Pauli exclusion principle). It is of short-range nature and thus it is enough to consider nearest-neighbor couplings.

NOTE: the exchange interaction should not be confused with the dipole-dipole interaction which is of long-range nature. In “*classical*” ferromagnets, like Fe and Ni, the dipolar interaction is much smaller than the exchange interaction and can be neglected unless one is considering temperatures very close to the Curie temperature (much closer than those obtained currently in labs). But, there are materials (for instance, some Gd compounds) in which dipolar interactions are important. In these systems, the critical behavior is different from that we are going to describe.

3. The terms proportional to D_{Is} and D_{cubic} are anisotropy terms that are due to the presence of a lattice structure.

4. Ising systems are those in which $D_{\text{Is}} < 0$, so that spins tend to align along the z -axis (uniaxial systems). In this case the critical modes are associated with the sign of the z -component of the spin. Thus, we can further simplify the Hamiltonian, assuming $\mathbf{S}_i = (0, 0, \sigma_i)$, $\sigma_i = \pm 1$. The Hamiltonian becomes (Ising Hamiltonian)

$$H = \sum J_{ij} \sigma_i \sigma_j$$

More formally: the critical behavior is independent of D_{Is} as long as D_{Is} is negative. Thus, we consider the limit $D_{\text{Is}} \rightarrow -\infty$. In this limit the identification is rigorous.

The critical behavior of Ising systems is well known and the critical exponents are known exactly in 2D and to high precision in 3D:

$$\begin{array}{llll} 2D : & \nu = 1 & \gamma = 7/4 & \beta = 1/8 \\ 3D : & \nu = 0.6301(4) & \gamma = 1.2372(5) & \beta = 0.3265(3) \end{array}$$

NOTE: For $D_{\text{Is}} = 0$ and $D_{\text{Is}} > 0$ we obtain a different critical behavior:

1. For $D_{\text{Is}} = 0$ we obtain a Heisenberg system (Fe and Ni are Heisenberg systems with good precision).
2. For $D_{\text{Is}} > 0$ spins magnetize in a plane orthogonal to the z -axis (easy plane) and the corresponding universality class is called *XY* universality class. In this case the relevant components are those in the xy plane and thus we can replace \mathbf{S}_i with a two-dimensional spin.

Heisenberg systems and *XY* systems have different critical exponents.

In 3D:

$$\begin{array}{llll} \text{XY} & \nu = 0.6716(3) & \gamma = 1.3177(5) & \beta = 0.3485(9); \\ \text{Heisenberg} & \nu = 0.7112(5) & \gamma = 1.3960(9) & \beta = 0.3689(3). \end{array}$$

Introducing the dilution

Consider a ferromagnetic system and introduce vacancies. In practice this can be obtained by replacing some of the magnetic atoms with nonmagnetic ones. For instance, iron difluoride FeF_2 and manganese difluoride MnF_2 are uniaxial antiferromagnets whose critical behavior is well described by the Ising universality class. A dilute material is obtained by replacing the magnetic ions with nonmagnetic ones, for instance with zinc, obtaining mixtures $\text{Fe}_x\text{Zn}_{1-x}\text{F}_2$.

QUESTION: Does the introduction of dilution change the universality class?

RESULTS FOR DILUTE ISING SYSTEMS

	material	concentration	γ	ν	α	β
(1986)	$\text{Fe}_x\text{Zn}_{1-x}\text{F}_2$	$x = 0.46$	1.33(2)	0.69(3)		
(1986)	$\text{Mn}_x\text{Zn}_{1-x}\text{F}_2$	$x = 0.75$	1.364(76)	0.715(35)		
(1988)	$\text{Fe}_x\text{Zn}_{1-x}\text{F}_2$	$x = 0.9$				0.350(9)
(1988)	$\text{Mn}_x\text{Zn}_{1-x}\text{F}_2$	$x = 0.40, 0.55, 0.83$			-0.09(3)	
(1988)	$\text{Mn}_x\text{Zn}_{1-x}\text{F}_2$	$x = 0.5$				0.33(2)
(1997)	$\text{Fe}_x\text{Zn}_{1-x}\text{F}_2$	$x = 0.5$				0.36(2)
(1998)	$\text{Fe}_x\text{Zn}_{1-x}\text{F}_2$	$x = 0.93$			-0.10(2)	
(1999)	$\text{Fe}_x\text{Zn}_{1-x}\text{F}_2$	$x = 0.93$	1.34(6)	0.70(2)		

Ising values:

$$\gamma = 1.2372(5) \quad \nu = 0.6301(4) \quad \alpha = 0.1096(5) \quad \beta = 0.3265(3).$$

Exponents are clearly different!! Dilution changes the universality class.

RESULTS FOR DILUTE HEISENBERG SYSTEMS

	Material	γ	β	δ
1994	Fe ₁₃ Ni ₆₇ Bi ₁₉ Si	1.386(12)	0.367(15)	4.50(5)
1994	Fe ₁₆ Ni ₆₄ Bi ₁₉ Si	1.386(14)	0.360(15)	4.86(4)
1995	Fe ₂₀ Ni ₆₀ P ₁₄ B ₆	1.386(10)	0.367(10)	4.77(5)
1995	Fe ₄₀ Ni ₄₀ P ₁₄ B ₆	1.385(10)	0.364(5)	4.79(5)
1997	Fe ₉₁ Zr ₉	1.383(4)	0.366(4)	4.75(5)
1997	Fe ₈₉ CoZr ₁₀	1.385(5)	0.368(6)	4.80(4)
1997	Fe ₈₈ Co ₂ Zr ₁₀	1.389(6)	0.363(5)	4.81(5)
1997	Fe ₈₄ Co ₆ Zr ₁₀	1.386(6)	0.370(5)	4.84(5)
1999	Fe _{1.85} Mn _{1.15} Si	1.543(20)	0.408(60)	4.74(7)
1999	Fe _{1.50} Mn _{1.50} Si	1.274(60)	0.383(10)	4.45(19)
1999	MnCr _{1.9} In _{0.1} S ₄	1.39(1)	0.36(1)	4.814(14)
1999	MnCr _{1.8} In _{0.2} S ₄	1.39(1)	0.36(1)	4.795(10)
2000	Fe ₈₆ Mn ₄ Zr ₁₀	1.381	0.361	
2000	Fe ₈₂ Mn ₈ Zr ₁₀	1.367	0.363	
2001	Fe ₈₄ Mn ₆ Zr ₁₀	1.37(3)	0.359	4.81(4)
2001	Fe ₇₄ Mn ₁₆ Zr ₁₀	1.39(5)	0.361	4.86(3)

Pure Heisenberg systems:

$$\gamma = 1.3960(9) \quad \beta = 0.3689(3) \quad \delta = 4.783(3).$$

Exponents are not different!! Dilution does not change the universality class.

HARRIS CRITERION

Consider a system with random dilution:

- If the **specific-heat** exponent α is **POSITIVE**, random dilution **CHANGES** the universality class of the pure system.
- If the **specific-heat** exponent α is **NEGATIVE**, random dilution **DOES NOT CHANGE** the universality class of the pure system.

CONSEQUENCES:

XY and Heisenberg systems have a negative specific-heat exponent. Hence, dilution does not change the leading critical behavior (but scaling corrections are different!).

Ising systems have a positive specific-heat exponent. Hence, dilution changes the leading critical behavior.

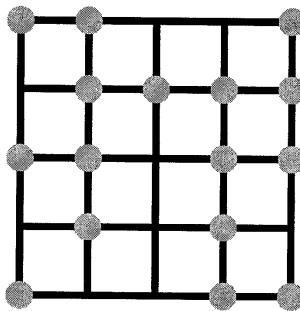
Interesting case: 2D Ising model.

In this case $\alpha = 0$ and the specific heat diverges logarithmically. Dilution is marginal and induces logarithmic corrections:

$$\xi \sim \frac{|t|^{-\nu}}{(-\log |t|)^{1/2}}, \quad \nu = 1$$

MODELS: the random-site dilute model

Consider the pure (Ising or XY or Heisenberg) model on a lattice (say cubic lattice) and randomly take out some spins. Physically, we are substituting magnetic ions with non-magnetic ones.



Hamiltonian:

$$H = - \sum_{\langle ij \rangle} \rho_i \rho_j \sigma_i \sigma_j$$

The sum is extended over all lattice nearest neighbors as in the usual Ising model.

ρ_i is the dilution variable that takes values $\rho_i = 1, 0$ with probability:

$$\text{Prob}(\rho_i) = P(\rho_i) = \begin{cases} p & \text{if } \rho_i = 1 \text{ (magnetic site);} \\ 1 - p & \text{if } \rho_i = 0 \text{ (empty, nonmagnetic site).} \end{cases}$$

In a pure system of course $p = 1$.

Averaging over disorder

Two possibilities: **Annealed** average, **Quenched** average.

- **Annealed**: the position of the vacancies is not fixed but evolves together with the spins.
- **Quenched**: the position of the vacancies is fixed (physically, this is the case if the diffusion time of the vacancies is much larger than the observation time).

The annealed case is relevant for magnetic fluids, while the quenched case is relevant for dilute (anti)ferromagnets.

In mathematical terms:

Annealed average: we average the **partition function** over disorder:

$$Z = \sum_{\{\rho_i\}} P(\rho_i) \sum_{\{\sigma_i\}} e^{-\beta H}, \quad F = -k_B T \ln Z.$$

Quenched average: we average the **free energy** over disorder:

$$Z(\{\rho_i\}) = \sum_{\{\sigma_i\}} e^{-\beta H}, \quad F(\{\rho_i\}) = -k_B T \ln Z(\{\rho_i\}),$$
$$F = \sum_{\{\rho_i\}} P(\rho_i) F(\{\rho_i\}).$$

The critical behavior of annealed systems is not very much different from that of pure systems. A model describing an Ising system with annealed dilution in the grand-canonical ensemble for the vacancies is the spin-1 (Blume-Emery-Griffiths) Ising model.

From now on we shall focus on **quenched systems**.

The random-bond Ising model:

$$H = - \sum_{\langle ij \rangle} J_{ij} \sigma_i \sigma_j, \quad J_{ij} = 1, 0 .$$

This is a model with a random hopping term, satisfying:

$$P(J_{ij}) = \begin{cases} p & J_{ij} = 1; \\ 1 - p & J_{ij} = 0. \end{cases}$$

The random-site and the random-bond models are particular instances of more general models. For instance, we expect the same critical behavior if we consider a random-site model in which the probability $P(\rho)$ has a finite support on the positive real axis,

$$P(\rho) = 0 \text{ for } \rho < 0 \text{ and } \rho > \rho_{\max},$$

and is otherwise arbitrary.

The condition that $P(\rho)$ vanishes for negative ρ guarantees a ferromagnetic low-temperature ground state (**But it is not a necessary condition, we will see it later**).

The condition $P(\rho) = 0$ for $\rho > \rho_{\max}$ can be replaced by the requirement that $P(\rho) \rightarrow 0$ for $\rho \rightarrow +\infty$ sufficiently fast.

In the random-site and in the random-bond models the probabilities of the vacancies on different sites (or different bonds) are uncorrelated. **This is not a necessary condition.** Short-range correlations are allowed.

An example is the **random-anisotropy model** with cubic symmetry, which is a random-bond Ising model with

$$J_{ij} = \vec{n}_i \cdot \vec{n}_j$$

and \vec{n}_i are random vectors defined on sites that can take the values: $(\pm 1, 0, 0)$, $(0, \pm 1, 0)$, $(0, 0, \pm 1)$.

Clearly, J_{ij} and J_{ik} (**same** i) are correlated, since they are obtained by using the same vector \vec{n}_i .

Mathematically, correlations can be characterized in terms of Wilson-loop averages.

Consider a square loop of size $L \times L$. Then,

$$W(L) = \left[\prod_{ij} J_{ij} \right] = 3^{1-L}$$

where:

the product is over the links belonging to the loop;

the symbol $[\cdot]$ denotes the average over the J_{ij} distribution.

Note that $W(L) \rightarrow 0$ **exponentially** for $L \rightarrow \infty$: correlations are short-ranged.

One can show that the the **random-anisotropy model** with cubic symmetry has a ferromagnetic low-temperature phase and that the transition is in the same universality class as that of the randomly dilute Ising model.

Back to the Harris criterion

We wish to understand the Harris criterion.

Let us consider the randomly dilute Ising model with a very small amount of dilution, i.e. for $1 - p \ll 1$. Let us rewrite the Hamiltonian as

$$H = \sum_{\langle ij \rangle} \rho_i \rho_j \sigma_i \sigma_j = H_{\text{pure}} + \sum_{\langle ij \rangle} (1 - \rho_i \rho_j) \sigma_i \sigma_j.$$

Let us now expand the partition function:

$$e^{-\beta H} = e^{-\beta H_{\text{pure}}} \left\{ 1 - \beta \sum_{\langle ij \rangle} (1 - \rho_i \rho_j) \sigma_i \sigma_j + \frac{1}{2} \beta^2 \left[\sum_{\langle ij \rangle} (1 - \rho_i \rho_j) \sigma_i \sigma_j \right]^2 + \dots \right\}$$

Since $[\rho_i] = p$, if $q = 1 - p^2$, we have for $q \ll 1$:

$$\frac{F}{V} = \frac{F_{\text{pure}}}{V} + qE - \frac{\beta q^2}{2} C_E + \dots$$

where:

$E = \langle \sigma_i \sigma_j \rangle$ is the energy in the pure model;

C_E is the specific heat in the pure model.

This expansion gives the free energy of the dilute model in terms of energy correlations in the pure model.

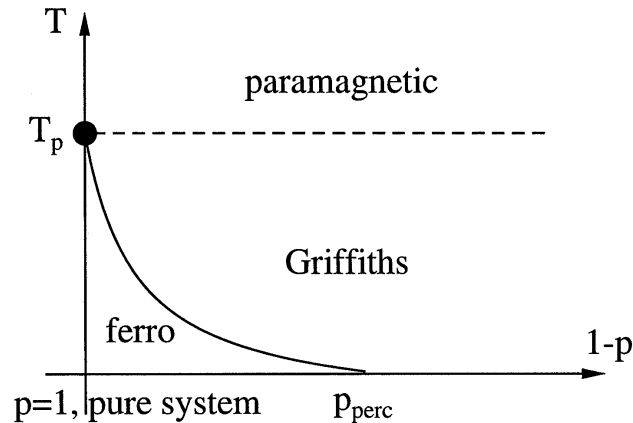
It explains why we shall often refer to dilution as **randomness coupled to the energy**.

It explains the Harris criterion. Indeed:

1. If corrections diverge we expect the critical behavior to be different from that of the pure model. If they vanish the critical behavior should be the same as that of the pure model.
2. If $\alpha > 0$, $C_E \rightarrow \infty$. Thus, $\alpha > 0$ implies that random dilution changes the universality class.
3. If $\alpha < 0$, corrections are finite. One can show that their only effect is a critical-temperature shift and different scaling corrections; however, the leading behavior is unchanged.

Phase diagram of dilute systems

The phase diagram of dilute systems has the following generic shape:



- In the low-temperature phase there is a ferromagnetic phase for $p > p_{\text{perc}}$, where p_{perc} is the percolation threshold of the spins. The absence of a ferromagnetic phase for $p < p_{\text{perc}}$ (large number of vacancies) is easy to understand: in this regime spin clusters do not percolate and form finite islands. Thus, there is no possibility for ferromagnetism.
- For $T = T_c(p)$, $1 \geq p \geq p_{\text{perc}}$, there is a paramagnetic-ferromagnetic transition line. Note that the critical temperature $T = T_c(p)$ decreases with decreasing p . It is easy to understand its origin. Due to the vacancies the effective number of neighbors decreases and thus the tendency to align decreases (think at the usual mean-field calculations).
- If $T_p = T_c(p = 1)$ is the critical temperature in the pure model, for $T > T_p$ there is a standard paramagnetic phase.
- The intermediate region

$$\begin{cases} T_c(p) < T < T_p & \text{for } p > p_{\text{perc}} , \\ 0 < T < T_p & \text{for } p < p_{\text{perc}} , \end{cases}$$

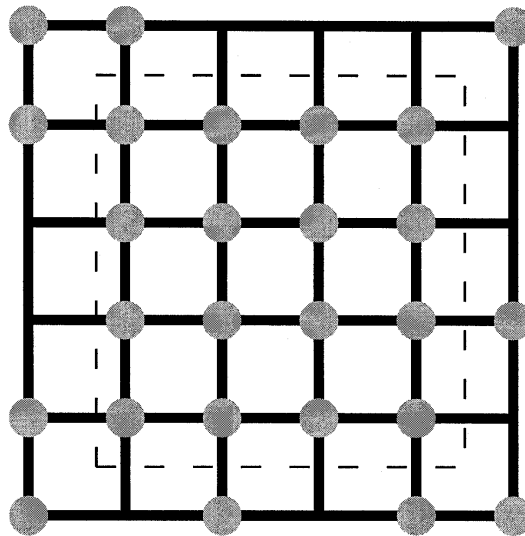
is called **Griffiths** phase. From the point of view of magnetic order, the Griffiths phase is paramagnetic. However, there are also some unusual features.

NOTE: There is at present no indication that the percolation threshold of the **vacancies** plays any role. Numerical works indicate that the critical transition and the phases do not depend on the geometric structure of the vacancies: it is not relevant if the vacancies percolate or not.

Properties of the Griffiths phase

This is an unusual phase that characterizes all random systems.

It is due to the fact that there are samples in which large space regions do not present vacancies (Griffiths islands) and which magnetize for $T < T_p$.



4 x 4 Griffiths island

The probability of a Griffiths island is exponentially small in the volume. Still, it has effects on the static and (more importantly) on the dynamic behavior.

STATIC BEHAVIOR: The free energy is not analytic in the Griffiths phase (theorem for Ising systems, believed to hold for XY and Heisenberg systems).

For instance, consider the free energy as a function of the magnetic field h . The free energy is not analytic for $h = 0$. These singularities are however quite weak. Indeed, the free energy is infinitely differentiable. Thus, it might be a singularity of the type

$$F(\beta, h) = F_{\text{analytic}}(\beta, h) + \exp(-a(\beta)/h), \quad a(\beta) > 0.$$

DYNAMIC BEHAVIOR: Griffiths islands are instead crucial for the dynamics (Bray, 1988).

The setting: consider a randomly dilute model and a local dynamics without conservation laws. This is the appropriate dynamics for Ising antiferromagnets.

Result: disorder-averaged autocorrelation functions **DO NOT** decay exponentially, as is expected in a paramagnetic phase.

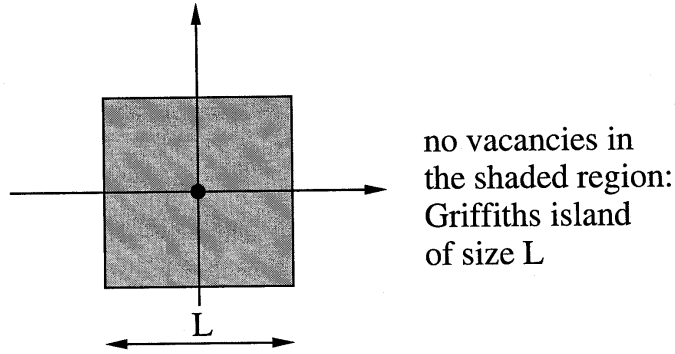
Derivation of the asymptotic behavior for Ising systems

Let us consider the disorder-averaged spin-spin autocorrelation function:

$$\begin{aligned} C(t) &= \overline{[\langle \sigma(x=0, t=0) \sigma(x=0, t) \rangle]} \\ &= \sum_{\{\rho_i\}} P(\{\rho_i\}) \langle \sigma(x=0, t=0) \sigma(x=0, t) \rangle_{\{\rho_i\}} \end{aligned}$$

For a reversible dynamics, the autocorrelation function is positive.

We can obtain a lower bound on $C(t)$ by considering only a particular set of samples: those that have a Griffiths island L^d centered in $x=0$.



$$C(t) \geq \sum P(L) \langle \sigma(x=0, t=0) \sigma(x=0, t) \rangle_L$$

Now:

- $P(L)$ is the probability of a block of size L centered in 0 with no vacancies. Since there are no site-site correlations, we have

$$P(L) = e^{-\alpha L^d}, \quad \alpha = -\ln p$$

$P(L)$ decays exponentially as $L \rightarrow \infty$, as expected.

- the dynamics is controlled (at least for large L) by the dynamics within the block. Since the block is magnetized (we are considering $T < T_p$) we have (Ising systems)

$$\langle \sigma(x=0, t=0) \sigma(x=0, t) \rangle_L \sim \exp(-t/\tau(L)), \quad \tau = \exp(\sigma L^{d-1}).$$

- Putting the terms together we obtain

$$C(t) \geq \sum_L \exp[-\alpha L^d - t \exp(-\sigma L^{d-1})].$$

We can evaluate the dominant term for $t \rightarrow \infty$, by computing the stationary point with respect to L .

If

$$f(L) = -\alpha L^d - t \exp(-\sigma L^{d-1}),$$

then

$$\frac{df}{dL} = 0, \quad \Rightarrow \quad L \sim (\ln t)^{1/(d-1)}$$

so that

$$C(t) \geq \exp[-A(\ln t)^{d/(d-1)}] \quad (d = 3) \quad C(t) \geq \exp[-A(\ln t)^{3/2}]$$

CONCLUSION: $C(t)$ does not decay exponentially.

NOTE: $C(t)$ decays faster than any power law.

Thus: the dynamics is slower than in a standard paramagnetic phase, but it is faster than that at a continuous phase transition.

Field theory

In mean-field theory the Ising behavior can be understood in terms of the Landau-Ginzburg Hamiltonian. Let Φ be the magnetization. Then we rewrite

$$\begin{aligned} Z &= \sum_{\{\sigma\}} e^{-\beta H[\sigma] - \sum_i h \sigma_i} = \sum_{\{\sigma\}} \sum_{\Phi} \delta \left(\Phi - \frac{1}{V} \sum_i \sigma_i \right) e^{-\beta H[\sigma] - \sum_i h \sigma_i} \\ &= \sum_{\Phi} e^{-V h \Phi - V H_{LG}(\Phi)}. \end{aligned}$$

where

$$e^{-V H_{LG}(\Phi)} = \sum_{\{\sigma\}} \delta \left(\Phi - \frac{1}{V} \sum_i \sigma_i \right) e^{-\beta H[\sigma]}.$$

The basic assumption of the Landau-Ginzburg theory is that $H_{LG}(\Phi)$ is well behaved so that one can expand it in powers of Φ :

$$H_{LG}(\Phi) = H_0 + A(T)\Phi^2 + B(T)\Phi^4 + \dots$$

For $V \rightarrow \infty$ only the value of Φ that minimizes $H_{LG}(\Phi)$ matters. A textbook calculation indicates that the minimum is obtained for

$$\Phi = \begin{cases} 0 & \text{if } A(T) > 0 \\ \Phi_0 \neq 0 & \text{if } A(T) < 0 \end{cases}$$

Here we assume $B(T) > 0$. If $B(T)$ is negative, we should also consider the Φ^6 term, obtaining a more complex behavior (tricritical points...)

The critical temperature T_c is defined by $A(T_c) = 0$.

The mean-field description misses a very important point:

FLUCTUATIONS: the local magnetization fluctuates wildly on the scale of the correlation length.

The correct critical behavior is only obtained by taking fluctuations into account.

How to introduce fluctuations in the LG theory:

1. replace the global magnetization Φ with a local magnetization $\phi(x)$.
2. introduce a fluctuation term

$$\frac{1}{2} \sum_{\mu} \left(\frac{\partial \phi}{\partial x_{\mu}} \right)^2 = \frac{1}{2} \sum_{\mu} (\partial_{\mu} \phi)^2.$$

Thus, the correct theory is given by

$$H = \int dx \left[\frac{1}{2} \sum_{\mu} (\partial_{\mu} \phi)^2 + \frac{r}{2} \phi^2 + \frac{\lambda}{4!} \phi^4 \right]$$

$$Z = \int [d\phi] e^{-H}$$

Note that the theory is defined in terms of a functional integral. Such an integral is not well defined mathematically and one needs a **regularization**.

A conceptually simple regularization is the *lattice* regularization.

We consider, e.g., a cubic lattice and replace

$$(\partial_{\mu} \phi)^2 \rightarrow (\phi(x + \hat{\mu}) - \phi(x))^2 = \phi(x + \hat{\mu})^2 + \phi(x)^2 - 2\phi(x + \hat{\mu})\phi(x)$$

Thus, we can replace

$$\sum_x \sum_{\mu} \frac{1}{2} (\partial_{\mu} \phi)^2 \rightarrow 3 \sum_x \phi(x)^2 - \sum_{\langle xy \rangle} \phi(x)\phi(y)$$

The Hamiltonian becomes

$$H = - \sum_{\langle xy \rangle} \phi(x)\phi(y) + \sum_x V(\phi_x), \quad V(\phi) = \frac{1}{2}(r + 6)\phi^2 + \frac{\lambda}{4!}\phi^4.$$

This Hamiltonian is an Ising Hamiltonian for “soft” spins. The Ising Hamiltonian is obtained in the limit

$$\lambda \rightarrow +\infty, \quad r \rightarrow -\infty, \quad \frac{r}{\lambda} \rightarrow -\frac{\beta}{6}.$$

Indeed, in this limit

$$V(\phi) = \frac{\lambda}{4!} (\phi^2 - \beta)^2$$

so that $e^{-V(\phi)}$ vanishes for $\lambda \rightarrow \infty$ unless $\phi^2 = \beta$. If we set $\phi = \sqrt{\beta}\sigma$, $\sigma = \pm 1$ we reobtain the Ising Hamiltonian.

Perturbation theory

In perturbation theory we expand in powers of λ for λ small. More precisely, perturbation theory is organized in powers of $\tilde{\lambda} = \lambda t^{-(4-d)/2}$ where $t = r - r_c(u)$ and $r_c(u)$ is fixed by the condition that the correlation length vanishes for $t = 0$.

To understand this point, let us start from the LGW Hamiltonian

$$H[\varphi] = \int dx \left[H\varphi + \frac{1}{2}(\partial\varphi)^2 + \frac{r}{2}\varphi^2 + \frac{\lambda}{4!}\varphi^4 \right].$$

Then, let us perform a change of variables. We consider a new field $\psi(s)$ defined by

$$\psi(s) = \lambda^\alpha \varphi(s\lambda^\beta).$$

Then, we fix α and β so that $H[\psi]$ can be written in the form:

$$H[\psi] = \int d^d s \left[\tilde{H}\psi + \frac{1}{2}(\partial\psi)^2 + \frac{\tilde{r}}{2}\psi^2 + \frac{1}{4!}\psi^4 \right],$$

NOTE: the coefficients of $(\partial\psi)$ and of ψ^4 are 1. This requirement gives two equations that allow us to obtain the exponents α and β :

$$\alpha = (d-2)/[2(d-4)] \qquad \beta = -1/(4-d).$$

The coefficients \tilde{H} and \tilde{r} are given by

$$\tilde{H} \equiv H\lambda^{-(d+2)/[2(4-d)]}, \qquad \tilde{r} \equiv r\lambda^{-2/(4-d)}.$$

Thus, formally, once the Hamiltonian is expressed in terms of ψ , the bare parameters appear only in the combinations \tilde{H} and \tilde{r} .

Since the free energy is invariant under field redefinitions, it depends only on \tilde{H} and \tilde{r} .

This derivation assumes scale invariance, which is not satisfied by the regularized theory. If one takes into account the breaking of scale invariance, one must make only one change:

replace r with $t = r - r_c(\lambda)$, where t vanishes at the critical transition and $r_c(\lambda)$ is a non-perturbative function.

The necessity of this renormalization is easy to understand. It expresses the fact that the critical behavior is not obtained for $r = 0$ as in the mean-field model or for $\lambda = 0$. For any given λ one should determine the critical value $r_c(\lambda)$.

Perturbation theory in terms of $\tilde{\lambda} = \lambda/t^{(4-d)/2}$ is not convenient: the critical limit is obtained for $t \rightarrow 0$, hence $\tilde{\lambda} \rightarrow \infty$. Thus, we should obtain the large- λ from the small- λ behavior.

Renormalized perturbation theory

The trick consists in expressing the perturbative series in terms of a renormalization-group invariant quantity. In perturbation theory one usually considers the **four-point renormalized coupling** g , but conceptually any renormalization-group invariant quantity could be used.

Define:

- **Correlation length:**

$$\xi^2 = \frac{1}{2d} \frac{\sum_x |x|^2 \langle \phi(0)\phi(x) \rangle}{\sum_x \langle \phi(0)\phi(x) \rangle}$$

This definition does not depend on the normalization of the fields and has the correct length dimensions. This is the standard definition of the *second-moment* correlation length used in numerical calculations.

- **Coupling g :**

$$g = \frac{\sum_{x,y,z} \langle \phi(0)\phi(x)\phi(y)\phi(z) \rangle^{\text{conn}}}{\xi^d [\sum_x \langle \phi(0)\phi(x) \rangle]^2}$$

The coupling g is RG invariant since:

1. it is invariant under field rescalings: the same number of fields appears in the numerator and in the denominator;
2. it is invariant under length rescalings:

$$\begin{aligned} \text{numerator} &\sim \int dx dy dz \sim (\text{length})^{3d} \\ \text{denominator} &\sim \xi^d \left(\int dx \right)^2 \sim (\text{length})^{3d} \end{aligned}$$

Now we have

$$g = \tilde{\lambda} + a_2 \tilde{\lambda}^2 + a_3 \tilde{\lambda}^3 + \dots$$

We then invert this expansion to obtain $\tilde{\lambda}$ as a function of g and express all quantities in terms of g .

To obtain critical results perturbative series should be computed at $g = g^*$, where g^* is the value of g at the critical point.

How do we determine g^* in perturbation theory?

β function and fixed points

On the lattice g and ξ are functions of the temperature β :

$$g = g(\beta), \quad \xi = \xi(\beta).$$

Of course we can also use ξ as independent variable and consider $g(\xi)$,

$$\text{given } \xi \rightarrow \beta \text{ by inverting } \xi = \xi(\beta) \rightarrow g(\xi) = g(\beta);$$

or use g as independent variable and consider $\xi(g)$.

The β -function is defined as

$$B(g) = -\xi \frac{dg}{d\xi}$$

and is always thought as a function of g .

Properties of $B(g)$ close to the critical point

For $\beta \rightarrow \beta_c$, g and ξ behave as

$$\begin{aligned} g &= g^* + a(\beta_c - \beta)^\Delta + \dots \\ \xi &= b(\beta - \beta_c)^{-\nu} [1 + c(\beta_c - \beta)^\Delta + \dots] \end{aligned}$$

Δ is a correction-to-scaling exponent which is universal and depends only on the universality class.

Explicitly, keeping only the leading term

$$\frac{dg}{d\xi} = \frac{dg/d\beta}{d\xi/d\beta} = \frac{-\Delta a(\beta_c - \beta)^{\Delta-1}}{\nu b(\beta_c - \beta)^{-\nu-1}} = -\frac{\Delta a}{\nu b} (\beta_c - \beta)^{\Delta+\nu}.$$

Thus, we obtain

$$B = \frac{\Delta a}{\nu} (\beta_c - \beta)^\Delta.$$

Finally, we must express it in terms of g :

$$g = g^* + a(\beta_c - \beta)^\Delta \Rightarrow \beta_c - \beta = \left(\frac{g - g^*}{a} \right)^{1/\Delta}$$

This gives finally

$$B(g) = \omega(g - g^*) + \dots, \quad \omega = \frac{\Delta}{\nu}$$

The β function satisfies the following properties:

1. It vanishes at the critical point (we say that $g = g^*$ is a fixed point).
2. It satisfies (**STABLE** fixed point):

$$\left. \frac{dB}{dg} \right|_{g=g^*} > 0$$

To understand the origin of this terminology, set $\xi = e^\tau$. The critical point is reached for $\tau \rightarrow \infty$ (in some sense τ is a “time”).

From the definition of the β function we have

$$\frac{dg}{d\tau} = -B(g)$$

This equation is usually called **flow** equation, since it controls how g varies with the time τ . Now note:

1. if $g = g^*$ at $\tau = 0$, we have $g = g^*$ for all $\tau > 0$; this is why g^* is called a fixed point;
2. if we start close to the fixed point

$$g(\tau) = g^* + Ae^{-\omega\tau},$$

where A depends on starting value. Since $\omega > 0$, for any starting condition $g(\tau) \rightarrow g^*$. Thus, g^* is a stable fixed point.

The strategy in field theory

1. Compute the perturbative expansion of g and ξ (and of any quantity of interest) in powers of $\tilde{\lambda}$.
2. Invert the previous relation to compute $\tilde{\lambda}$ in powers of g . All quantities of interest are expressed in terms of g .
3. Compute the β function and determine its zeros. Select the stable fixed point g^* .
4. Compute all quantities at $g = g^*$.

A technical problem: perturbative expansions in field theory are not convergent. Still they are Borel summable and this allows us to obtain finite results.

For pure models field theory gives results that have been competitive with numerical ones for a long time.

Field theory for random dilute Ising models

For the pure model, field theory (FT) is based on the Hamiltonian

$$H = \int dx \left[\frac{1}{2} \sum_{\mu} (\partial_{\mu} \phi)^2 + \frac{r}{2} \phi^2 + \frac{\lambda}{4!} \phi^4 \right]$$

How do we introduce randomness?

We know that in randomly dilute models, randomness is **coupled to the energy**.

Which is the correct coupling in FT?

The argument:

In the Ising model the energy is $E_x = \sigma_x \sigma_{x+\mu}$.

In the FT model we may consider $E_x = \phi_x \phi_{x+\mu}$.

Note, however, that the relevant length scale is the correlation length; thus, operators that differ on the scale of a single lattice spacing behave analogously (unless constraints are present).

Thus, we can take $E_x = \phi_x^2$.

For instance, in the lattice ϕ^4

$$\langle \phi^2(0) \phi(x)^2 \rangle^{\text{conn}} \sim t^{-\alpha},$$

as expected for the specific heat.

In order to introduce randomness we consider a space-dependent function $\psi(x)$ and add a term

$$\int dx \psi(x) \phi(x)^2$$

to the Hamiltonian, assuming where $\psi(x)$ to be normally distributed

$$P(\psi) \sim \exp(-\beta \psi^2).$$

The Hamiltonian is therefore

$$H = \int dx \left[\frac{1}{2} \sum_{\mu} (\partial_{\mu} \phi)^2 + \frac{r + \psi(x)}{2} \phi^2 + \frac{\lambda}{4!} \phi^4 \right],$$

Then, we define

$$Z[\psi] = \int [d\phi] e^{-H[\psi]}$$

and

$$\beta F = - \int [d\psi] P(\psi) \ln Z[\psi]$$

NOTE: Since we are considering quenched averages, we must average $\ln Z[\psi]$.

As it stands, perturbation theory is impossible. The way out is the **REPLICA TRICK**.

For $n \rightarrow 0$ (n real) we have

$$x^n = e^{n \ln x} \approx 1 + n \ln x \quad \Rightarrow \quad \ln x = \frac{1}{n}(x^n - 1).$$

Thus, we rewrite

$$\beta F = - \lim_{n \rightarrow 0} \frac{1}{n} \int [d\psi] P(\psi) (Z[\psi]^n - 1).$$

In practice, we should compute

$$G(n) = \int [d\psi] P(\psi) Z[\psi]^n$$

for REAL n and then take the limit $n \rightarrow 0$.

We shall compute $G(n)$ only for **INTEGER** values of n and then extrapolate to $n \rightarrow 0$. This is a dangerous procedure. In the spin-glass mean-field case this is incorrect (Parisi solution); in the randomly dilute models there is no evidence that this procedure fails.

The quantity $Z(\psi)^n$ can be rewritten as follows. Consider an n -dimensional field ϕ_a , $a = 1, \dots, n$ and define

$$H_n = \int dx \sum_a \left[\frac{1}{2} \sum_\mu (\partial_\mu \phi_a)^2 + \frac{1}{2}(r + \psi)\phi_a^2 + \frac{\lambda}{4!}\phi_a^4 \right]$$

Different components do not interact and therefore

$$Z[\psi]^n = \int [d\phi] e^{-H_n}.$$

In order to compute $G(n)$ we should average over disorder:

$$G[n] = \int [d\phi] \exp \left[\int dx \sum_a \left(\frac{1}{2} \sum_\mu (\partial_\mu \phi_a)^2 + \frac{r}{2}\phi_a^2 + \frac{\lambda}{4!}\phi_a^4 \right) \right] \\ \times \int [d\psi] \exp \left[\int dx \left(-\frac{1}{2}\psi \left(\sum_a \phi_a^2 \right) - \beta\psi^2 \right) \right]$$

The integral over the noise is a Gaussian integral that can be easily performed by a shift. Since:

$$-\frac{1}{2}\psi \left(\sum_a \phi_a^2 \right) - \beta\psi^2 = -\beta \left(\psi + \frac{1}{4\beta} \sum_a \phi_a^2 \right)^2 + \frac{1}{16\beta} \left(\sum_a \phi_a^2 \right)^2$$

the integral over ψ gives

$$\text{constant} \times \exp \left[\int dx \frac{1}{16\beta} \left(\sum_a \phi_a^2 \right)^2 \right].$$

This term couples the different components (replicas) and can be added to the Hamiltonian obtaining:

$$G[n] = \int [d\phi] \exp \left[\int dx \sum_a \left(\frac{1}{2} \sum_\mu (\partial_\mu \phi_a)^2 + \frac{r}{2}\phi_a^2 + \frac{\lambda}{4!}\phi_a^4 + \frac{\mu}{4!} \left(\sum_a \phi_a^2 \right)^2 \right) \right],$$

where we set $\mu/4! = -1/(16\beta)$.

Perturbation theory for the theory with replicas is standard and is derived from this Hamiltonian.

NOTE: there are two quartic couplings and this makes the treatment (slightly) more complex.

Strategy of the calculation

1. Compute the quantities of interest in terms of $\tilde{\lambda} = \lambda t^{-(4-d)/2}$, $\tilde{\mu} = \mu t^{-(4-d)/2}$.
2. Consider two renormalized couplings g_1 and g_2 that behave as $\tilde{\lambda}$ and $\tilde{\mu}$ at lowest order. The natural candidates are associated with the two independent 4-point correlation functions:

$$\begin{aligned} &\langle \phi^a(0)\phi^a(x)\phi^a(y)\phi^a(z) \rangle \\ &\langle \phi^a(0)\phi^a(x)\phi^b(y)\phi^b(z) \rangle \quad a \neq b \end{aligned}$$

3. Compute the corresponding TWO β functions and determine the fixed points. To determine their stability consider the Jacobian matrix

$$J = \frac{\partial(B_1, B_2)}{\partial(g_1, g_2)}.$$

A fixed point is stable if the eigenvalues of J are positive.

Results

An analysis of the perturbative expansions shows:

1. The Ising fixed point $(g_1^*, g_2 = 0)$ is **UNSTABLE**.
2. There is a new fixed point (g_1^*, g_2^*) which is **STABLE**.
3. This fixed point should be associated with the critical behavior in the presence of dilution.

Perturbative theory provides relatively precise estimates of the critical exponents that compare well with the numerical estimates.

	Method	γ	ν	η	ω
(2000)	$d = 3$ exp. $O(g^6)$	1.330(17)	0.678(10)	0.030(3)	0.25(10)
(2000)	$d = 3$ exp. $O(g^5)$	1.325(3)	0.671(5)	0.025(10)	0.32(6)
(1999)	$d = 3$ MS $O(g^4)$	1.318	0.675	0.049	0.39(4)
(2007)	MC	1.341(5)	0.683(2)	0.036(1)	0.29(2)

NOTE: ω which is the correction-to-scaling exponent is particularly **SMALL** (in pure systems $\omega \approx 0.8$).

Field theory for XY and Heisenberg dilute systems

The whole treatment can be extended to XY and Heisenberg dilute systems. In the pure system the basic variable is a vector field ϕ_α with $\alpha = 1, 2$ or $\alpha = 1, 2, 3$.

In the random case we should add a replica index. The basic field is $\phi_{a\alpha}$, $a = 1, \dots, n$.

The derivation of the Hamiltonian is the same.

RESULTS:

1. The pure fixed point $(g_1^*, g_2 = 0)$ is **STABLE**.
2. There is a new fixed point (g_1^*, g_2^*) , but it is **UNSTABLE**.

These results confirm the conclusions obtained by using the Harris criterion.

Field theory also predicts scaling corrections proportional to

$$|\beta - \beta_c|^{-\alpha}.$$

In the XY and Heisenberg case α is very small:

XY systems: $\alpha = -0.015$;

Heisenberg systems: $\alpha = -0.13$.

The asymptotic behavior is difficult to observe with good precision.

NUMERICAL WORKS: SOME COMMENTS

Field theory identifies a single universality class for randomly dilute systems and thus it predicts that the critical behavior is independent of the dilution.

Can we verify this statement numerically?

An UNBIASED test is VERY DIFFICULT.

Field theory predicts the leading and the next-to-leading correction-to-scaling exponents: $\omega \approx 0.3$, $\omega_2 \approx 0.8$. They are very small and thus many correction-to-scaling terms must be taken into account. For instance, for the susceptibility at the critical point we should consider a fit like

$$\chi(L) = aL^{2-\eta}(1 + b_1L^{-\omega} + b_2L^{-2\omega} + b_3L^{-3\omega} + b_4L^{-\omega_2})$$

In the pure model, incorrect results are obtained if we do not include the leading term $L^{-0.8}$, which is of the same order of $L^{-3\omega}$ and $L^{-\omega_2}$.

Of course, such a fit cannot be performed with the lattice sizes available today.

What can be done is a **consistency check**:

1. Assume that FT is correct and determine convenient models that minimize corrections. In practice we change the dilution parameter p until the scaling corrections decay as $L^{-\omega_2} \sim L^{-0.8}$. We call these models **improved models**.
2. For these models we compute numerically critical exponents and other universal quantities.
3. We consider several improved models and verify that the estimates obtained for the different models agree within errors.
4. Then, we consider generic values of the dilution parameter and verify that the observed behavior is *consistent* with a single universality class.

We have applied this strategy to the random-bond and to the random-site Ising model.

We have determined the improved Hamiltonian:

The random-site model is improved for $p = 0.80$;

The random-bond model is improved for $p = 0.54$.

NOTE: For $p = 0.80$ site vacancies do not percolate; for $p = 0.54$ bond vacancies percolate. The equality of the critical behavior indicates that the geometric structure of the vacancies is irrelevant.

RESULTS:

$$\nu = 0.683(2)$$

$$\eta = 0.036(1)$$

$\pm J$ Ising model

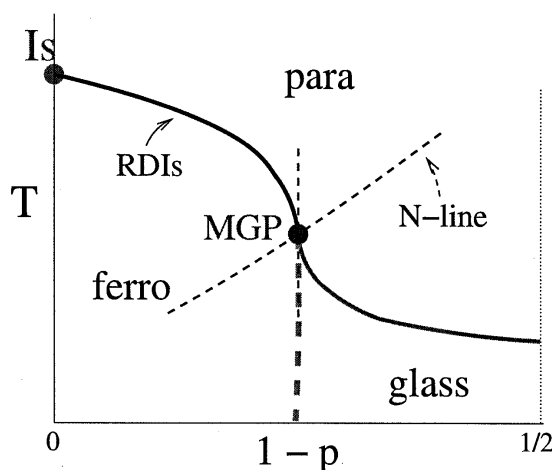
In the random-bond Ising model, J_{ij} assumes the values 0,1. A related model is the Edwards-Anderson model in which J_{ij} assumes the values $-1, 1$:

$$H = - \sum_{\langle ij \rangle} J_{ij} \sigma_i \sigma_j, \quad J_{ij} = 1, -1.$$

$$P(J_{ij}) = \begin{cases} p & J_{ij} = 1; \\ 1 - p & J_{ij} = -1. \end{cases}$$

This models describes the critical behavior of systems with ferromagnetic-antiferromagnetic couplings.

The phase diagram is the following:



We only report the magnetic transitions. We have not indicated the Griffiths phase, which is present for $T < T_{\text{Is}}$.

For a small amount of antiferromagnetic bonds, the system shows a para-ferro transition. This transition is in the same universality class of that of randomly dilute models, even though the Hamiltonian is not ferromagnetic (frustration is irrelevant).

For a larger amount of antiferromagnetic bonds there is a glassy phase and a paramagnetic-glassy transition. The nature of the transition does not depend on p and thus the critical behavior is the same as that of the bimodal spin-glass Ising model with $p = 1/2$.

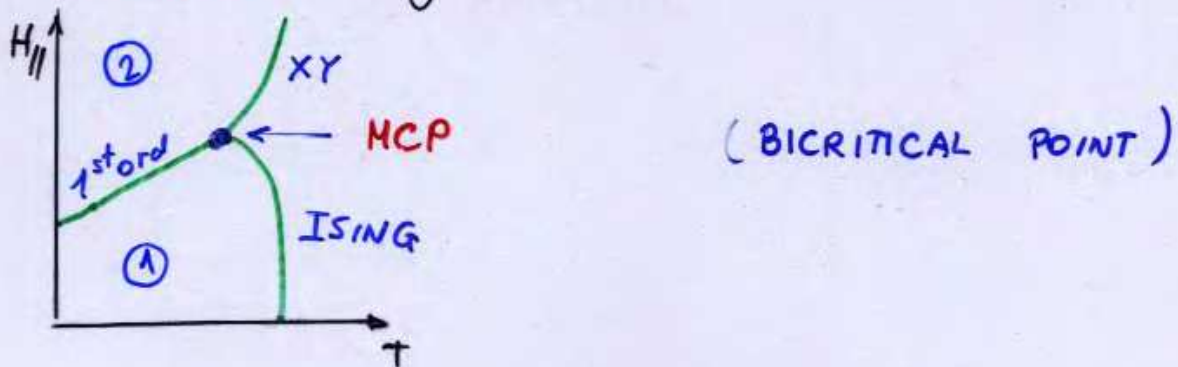
MULTICRITICAL POINTS

①

Multicritical points occur when critical lines associated with different order parameters meet

AN EXAMPLE: ISING ANTIFERROMAGNETS IN A UNIFORM MAGNETIC FIELD (CUBIC L)

It is equivalent to an Ising **FERROMAGNET** in a **STAGGERED** magnetic field



At the MCP three phases meet:

1. Ising ferromagnetic phase: $\vec{S} \parallel \hat{z}$
2. XY ferromagnetic phase: \vec{S} in xy plane
3. paramagnetic

OTHER TYPES OF MCP'S:



TETRACRITICAL MCP



PENTACRITICAL MCP

CRITICAL BEHAVIOR

In the standard Ising model the singular part of the free energy can be written as

$$F_{\text{sing}}(t, h) = u_t^{dv} f(u_h u_t^{-y_h/y_t}) + \text{scal. corrections}$$

u_h, u_t NON-LINEAR SCALING FIELDS

$$u_h = h (1 + a_1 t + a_2 t^2 + \dots + b_1 h^2 + \dots)$$

$$u_t = t (1 + c_1 t + c_2 t^2 + \dots + d_1 h^2 + \dots)$$

The scaling fields are ANALYTIC functions of the system parameters. At leading order

$$u_h \sim h \quad u_t \sim t$$

The absence of mixing terms is due to the $h \leftrightarrow -h$ symmetry of the Hamiltonian.

In the absence of symmetries, at leading order the scaling fields are LINEAR COMBINATIONS of the system parameters.

FLUID: (liquid-vapor)

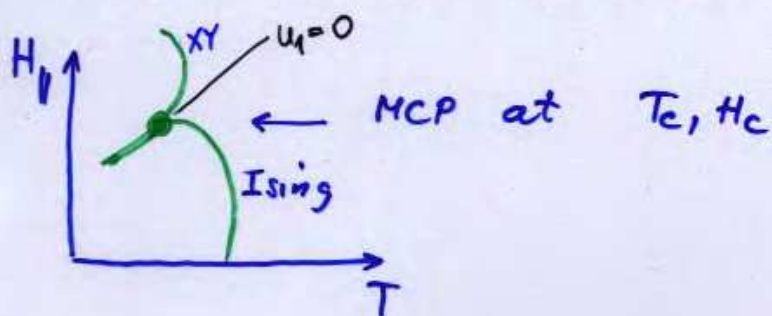
$$\begin{cases} u_h = \alpha \mu + \beta t \\ u_t = \gamma \mu + \delta t \end{cases}$$

+ (pressure?)

(NE Fisher's recent claim)

μ = chemical potential

BACK TO THE UNIAXIAL AF IN H FIELD ③



In this case there is no symmetry.

Hence, around the MCP the scaling fields are

$$u_1 = \alpha(H - H_c) + \beta(T - T_c)$$

$$u_2 = \gamma(H - H_c) + \delta(T - T_c)$$

$$F_{\text{sing}} = u_1^{d\nu} F(u_2 u_1^{-\phi})$$

ϕ = crossover exponent > 1

IMPORTANT PROPERTY:

All transition lines are tangent to $u_1 = 0$

Close to the MCP they satisfy

$$u_2 = \alpha_{\text{IS}} u_1^{\phi}$$

$$u_2 = \alpha_{\text{XY}} u_1^{\phi}$$

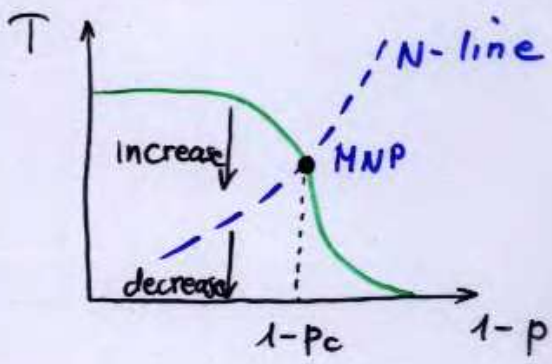
NISHIMORI LINE

In the $\pm J$ Ising model there is a very special line, called Nishimori line

$$\tanh \beta = 2p - 1$$

1. $\overline{\langle \sigma_0 \sigma_x \rangle} = \overline{\langle \sigma_0 \sigma_x \rangle^2}$
- ↑
correl. function
magnetic criticality
- ↑
correl. function
for SG criticality
(overlap correlation funct.)

2. At fixed p , ferromagnetic order is maximal along the N-line



It implies no ferromagnetic order for $p < p_c$



The MNP is a multicritical point where 3 phases meet

OPEN PROBLEM: FERRO-SG BOUNDARY

Mixed phase? Transition order? p -dependence?

FIELD THEORY RESULTS

Scaling fields:

$$u_1 = \alpha_1 (p - p_c) + \beta_1 (T - T_c)$$

$$u_2 = \alpha_2 (p - p_c) + \beta_2 (T - T_c)$$

RG dimensions y_1, y_2 satisfy $y_1 > y_2$

⇒ Critical lines are tg. to $u_1 = 0$

1. The Nishimori line is associated with a scaling field, i.e. either $u_1 = 0$ or $u_2 = 0$

Critical lines are not tangent to the N-line

↓

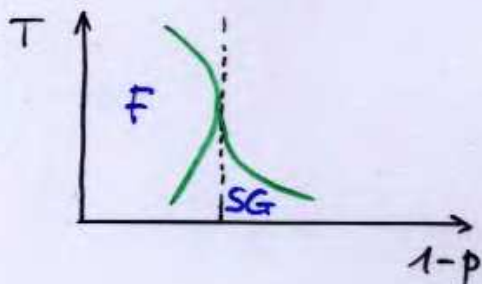
$$u_2 = 0$$

↓

$$u_2 = \tanh \beta - 2p + 1$$

2. In $6 - \epsilon$ dimensions

$$u_1 = p - p_c \quad (\text{NO MIXING})$$



All these results have been confirmed by MC simulations

Bias correction in simulations of disordered systems

Let us consider (for instance) the random-site Ising model and let us set $\pi(\sigma; \rho) = e^{-\beta\mathcal{H}}/Z$.

We wish to compute averages of functions $A(\sigma, \rho)$ that depend on the spins and on the dilution variables, for instance

$$\mathcal{O}_n \equiv \overline{\langle A \rangle^n} = \sum_{\rho} p(\rho) \left[\sum_{\sigma} \pi(\sigma; \rho) A(\sigma, \rho) \right]^n.$$

A possible numerical strategy:

- Extract N_s independent disorder configurations ρ_α , $\alpha = 1, \dots, N_s$, with probability $p(\rho)$ and then, for each ρ_α , extract N_m *independent* configurations $\sigma_{a,\alpha}$, $a = 1, \dots, N_m$, with probability $\pi(\sigma; \rho_\alpha)$. This is exactly the procedure used in MC simulations. N_s is the number of samples, N_m the number of measures per sample.
- Then, define the sample average

$$[A]_{\rho_\alpha} \equiv \frac{1}{N_m} \sum_{a=1}^{N_m} A(\sigma_{a,\alpha}, \rho_\alpha). \quad (1)$$

- A possible estimator of \mathcal{O}_n could be

$$\mathcal{O}_n^{\text{est}} \equiv \frac{1}{N_s} \sum_{\alpha=1}^{N_s} [A]_{\rho_\alpha}^n. \quad (2)$$

QUESTION: does $\mathcal{O}_n^{\text{est}}$ converge to \mathcal{O}_n as $N_s \rightarrow \infty$ at **FIXED** N_m .

One can show that, for $N_s \rightarrow \infty$ at fixed N_m , we have

$$\mathcal{O}_n^{\text{est}} \rightarrow \overline{\langle [A]^n \rangle}.$$

This is intuitive. The quantity we are really computing is the sample mean $[A]$; thus, by taking the limit $N_s \rightarrow \infty$ we average over the disorder distribution.

Now let us compute $\langle [A]^n \rangle$ for a given disorder distribution.

Case $n = 1$:

$$\langle [A] \rangle_\rho = \frac{1}{N_m} \left\langle \sum_{a=1}^{N_m} A(\sigma_a, \rho) \right\rangle_\rho = \langle A \rangle_\rho,$$

$\mathcal{O}_1^{\text{est}}$ converges to \mathcal{O}_1 irrespective of N_m : one could even take $N_m = 1$.

Case $n = 2$:

$$\begin{aligned} \langle [A]^2 \rangle_\rho &= \frac{1}{N_m^2} \left\langle \sum_{a=1}^{N_m} \sum_{b=1}^{N_m} A(\sigma_a, \rho) A(\sigma_b, \rho) \right\rangle_\rho \\ &= \frac{1}{N_m^2} \left[N_m(N_m - 1) \langle A \rangle_\rho^2 + N_m \langle A^2 \rangle_\rho \right] \\ &= \langle A \rangle_\rho^2 + \frac{1}{N_m} \left(\langle A^2 \rangle_\rho - \langle A \rangle_\rho^2 \right). \end{aligned}$$

$\mathcal{O}_2^{\text{est}}$ **DOES NOT** converge to \mathcal{O}_2 . The second term is what we called the **BIAS**.

Strategies to deal with the bias

(Naive approach) One possible approach consists in taking N_m large. This is not a good choice in high-precision studies.

(Parisi et al. approach) If \mathcal{O}^{est} is an estimator of $\bar{\mathcal{O}}$, which, for $N_s \rightarrow \infty$ at fixed N_m , converges to

$$\bar{\mathcal{O}} + \frac{a}{N_m} + O(1/N_m^2).$$

consider

$$\mathcal{O}^{\text{est,unb}} = 2\mathcal{O}^{\text{est}} - \frac{1}{2}\mathcal{O}_{1/2,1}^{\text{est}} - \frac{1}{2}\mathcal{O}_{1/2,2}^{\text{est}}.$$

Here \mathcal{O}^{est} is determined by using all N_m measures, while $\mathcal{O}_{1/2,1}^{\text{est}}$ and $\mathcal{O}_{1/2,2}^{\text{est}}$ are computed by using the first half and the second half of the measures.

Indeed:

$$\begin{aligned} 2\mathcal{O}^{\text{est}} &\rightarrow 2\bar{\mathcal{O}} + \frac{2a}{N_m} \\ \frac{1}{2}\mathcal{O}_{1/2,1}^{\text{est}} &\rightarrow \frac{1}{2}\bar{\mathcal{O}} + \frac{1}{2}\frac{a}{N_m/2} = \frac{1}{2}\bar{\mathcal{O}} + \frac{a}{N_m} \\ \frac{1}{2}\mathcal{O}_{1/2,2}^{\text{est}} &\rightarrow \frac{1}{2}\bar{\mathcal{O}} + \frac{1}{2}\frac{a}{N_m/2} = \frac{1}{2}\bar{\mathcal{O}} + \frac{a}{N_m} \end{aligned}$$

Summing up, we check that $1/N_m$ corrections vanish.

The advantage of this method is its generality; moreover it can be improved systematically.

(our approach) For products of thermal averages one can define estimators with **no bias**.

Divide the N_m configurations in n bunches and define the sample average over bunch i of length N_m/n :

$$[A]_{1/n,i,\rho_\alpha} \equiv \frac{n}{N_m} \sum_{a=1+(i-1)N_m/n}^{iN_m/n} A(\sigma_{a,\alpha}, \rho_\alpha). \quad (3)$$

A new estimator of \mathcal{O}_n is

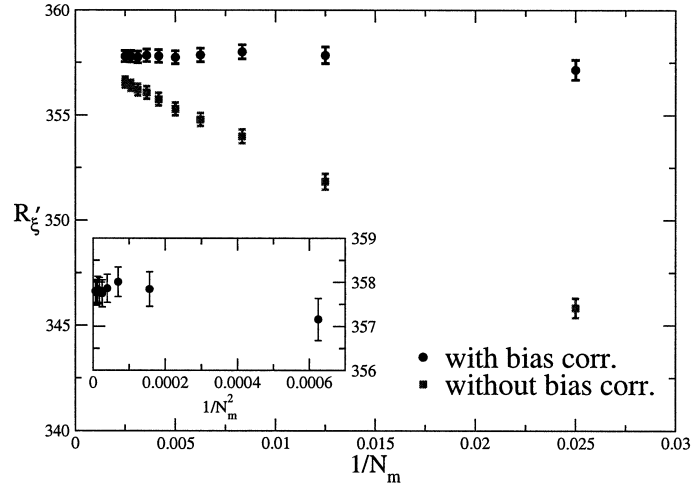
$$\mathcal{O}_n^{\text{unbiased}} \equiv \frac{1}{N_s} \sum_{\alpha=1}^{N_s} [A]_{1/n,1,\rho_\alpha} [A]_{1/n,2,\rho_\alpha} \cdots [A]_{1/n,n,\rho_\alpha}. \quad (4)$$

If correlations are present, it is easy to generalize these results: to compute $\overline{\langle A \rangle^2}$, we use

$$\frac{4}{N_s(N_m - 2k)^2} \sum_{\alpha=1}^{N_s} \sum_{i=1}^{N_m/2-k} A_{\alpha,i} \sum_{j=N_m/2+k}^{N_m} A_{\alpha,j}.$$

with k of the order of a few autocorrelation times.

Is it really necessary to take into account the bias correction?



R'_ξ for a run of the RSIM model at $L = 64$, $p = 0.8$, $N_s = 60000$, $\beta_{\text{run}} = 0.285742$, reweighted at $R_\xi = 0.5943$ as a function of $1/N_m$. In the insets we show the results for the bias-corrected estimates versus $1/N_m^2$. We report data with $N_m = 40, 80, 120, \dots, 400$.