UNIVERSITÀ DEGLI STUDI DI MILANO

Advanced Statistical Physics

Lecture 3

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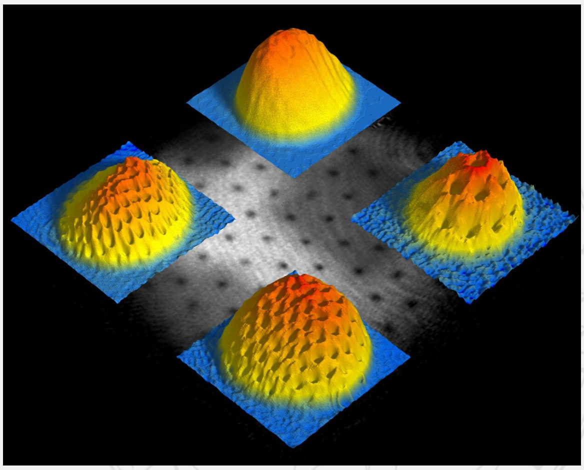

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Outline

- Spin models: Ising, XY, Heisenberg
- Mean field approximation for magnets
- Mean field critical exponents
- 1D Ising model: exact solution
- 1D Ising model: spin correlations
- 2D Ising model: free energy argument

Scope:

to point out limitations of the mean-field approximation in predicting the transition temperature and the critical exponents in low dimensions, by comparing with the exact solutions for the Ising model in 1D and 2D

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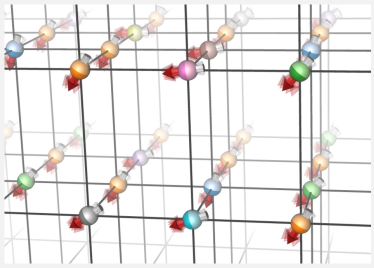
A model of phase transitions

- We find it convenient to formulate models of phase transitions in the language of ferromagnetism;
- We thus regard each of the N lattice sites to be occupied by an atom possessing a magnetic moment μ, of magnitude $g\mu_B\sqrt{[J(J+1)]}$, which is capable of (2J+1) discrete orientations in space, where J is the quantum number associated with the total angular momentum (orbital+spin): **J** := **L** + **S**



- These orientations define "different possible manners of occupation" of a given lattice site; accordingly, the whole lattice is capable of $(2J+1)^N$ different configurations.
- In a "classical" model for magnets J→∞ and the spins can take any direction in space: this is the classical Heisenberg model ↳ infinite orientazioni
- Associated with each configuration there is an energy E that arises from mutual interactions among the neighbouring atoms of the lattice and from the interaction of the whole lattice with an external field

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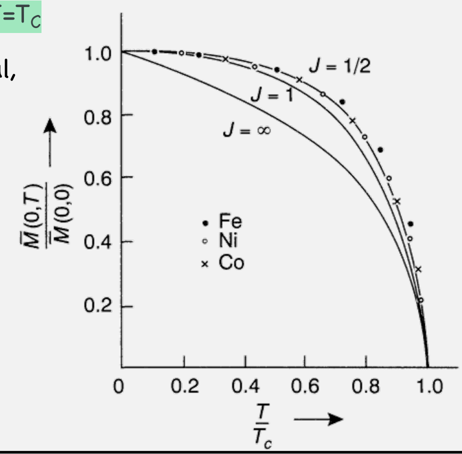
fase magnetizzata per $T<T_c$ ⇒ non per $T>T_c$
sempre a $H=0$

- A statistical analysis in the canonical ensemble should then enable us to determine the expectation value of the net magnetization, M
- The presence of a spontaneous magnetization at temperatures below a certain (critical) temperature T_C and its absence above that temperature will then be interpreted as a ferromagnetic phase transition in the system at $T=T_C$
- Detailed studies, both theoretical and experimental, have shown that, for many ferromagnetic materials, data on the temperature dependence of the spontaneous magnetization fit best with the value J=1/2
- Therefore, in discussing the problem of ferromagnetism, we may specifically start by taking: $\mu=g\mu_B\sqrt{[s(s+1)]}$, where s is the quantum number associated with the electron spin



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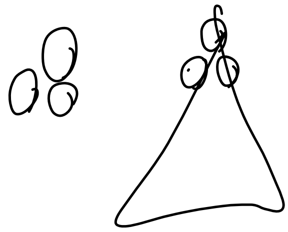
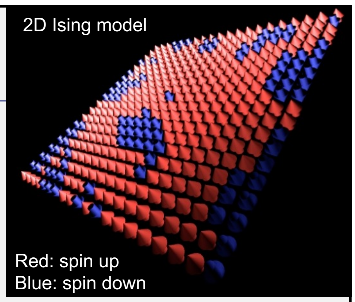


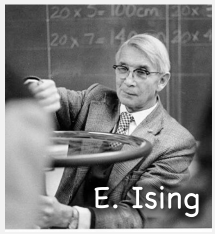
11/03/25

→ nella trattazione con tutte le interazioni non rientra la dimensionalità d → viene fuori introducendo i primi vicini

The classical Ising model



- With s=1/2, only two orientations are possible for each lattice site, namely $s_z = +1/2$ (with $\mu_z=+\mu_B$) and $s_z = -1/2$ (with $\mu_z=-\mu_B$). The whole lattice is then capable of 2^N configurations; one such configuration is shown in this picture for a 2D model
- This is the classical Ising model, the most famous model of statistical mechanics. It was invented by W. Lenz (1920), who proposed it as a thesis to one of his students (E. Ising).



- The energy of a configuration is measured by :

$$\boxed{E = -\tfrac{1}{2}\sum_{i,j=1}^{N} J_{ij}\sigma_i\sigma_j - h\sum_{i=1}^{N}\sigma_i}$$

ISING ESATTA

- Where: $\sigma_i \equiv$ component z of the magnetic moment of an electron; $h \equiv$ applied magnetic field; $J_{ij} \equiv$ tendency of electrons to align themselves parallel (or anti-parallel) because of the exchange interaction

è un caso di Heisenberg in cui $\hat{S}_z$ domina su x e y → il contrario è il modello di XY
↳ rotazione

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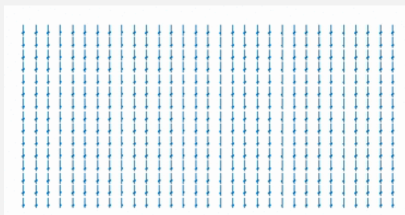
The exchange interaction

- Typically, the exchange interaction falls off rapidly as the separation of the two spins is increased. We may regard it as negligible for all but nearest-neighbor pairs:

$$E = -\tfrac{1}{2}J\sum_{\langle i,j\rangle_{n.n.}}\sigma_i\sigma_j - h\sum_{i=1}^{N}\sigma_i \quad \text{PRIMI VICINI}$$

J>0 tends to favour parallel spins, i.e. a model for ferromagnetism; J<0 favours anti-parallel spins, i.e. a model for anti-forromagnetism

- A different model results if we suppress the z-components of the spins and retain the x- and y-components instead. This model was originally introduced by Matsubara and Matsuda as a model with possible relevance to the superfluid transition in liquid ^{4}He; it is called the XY model



vortex-antivortex pair in a 2D XY model

- It seems appropriate to regard the Ising and the X-Y models as special cases of the anisotropic Heisenberg model with interaction parameters J_x, J_y and J_z; while the Ising model represents the situation J_x, J_y << J_z, the X-Y model represents just the opposite.

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non è la dimensione
→ infatti tutti e 3 i modelli possono vivere in spazio d-dimensionale

Role of dimensionality

- Introducing a parameter n, which denotes the number of spin components, we may regard the Ising, the XY and the Heisenberg models as pertaining to the n-values 1, 2 and 3, respectively.
- As we shall see, the parameter n, along with the dimensionality of the lattice, constitutes the basic set of elements that determine the qualitative nature of the critical behavior of a given system
- Rigorously speaking, spins are quantum mechanical operators and we have to justify the classical treatment introduced so far

Number of components	Hamiltonian
Heisenberg n = 3	$-\sum_{i<j} J_{ij}\vec{s}_i\cdot\vec{s}_j - \sum_i \vec{h}\cdot\vec{s}_j$ $\vec{s}_i = (\sin\vartheta_i\cos\varphi_i;\sin\vartheta_i\sin\varphi_i;\cos\vartheta_i)$ $\varphi_i\in[0,2\pi]\quad \vartheta_i\in[0,\pi]$
XY n = 2	$-\sum_{i<j} J_{ij}\vec{s}_i\cdot\vec{s}_j - \sum_i \vec{h}\cdot\vec{s}_j$ $\vec{s}_i = (\cos\vartheta_i;\sin\vartheta_i)\quad \vartheta_i\in[0,2\pi]$
Ising n = 1	$-\sum_{i<j} J_{ij}\sigma_i\sigma_j - h\sum_i \sigma_j$ $\sigma_i = \pm 1\ \forall i$

- An intuitive reason is that magnetic phases are caused by cooperation of very large incoherent number of microscopic degrees of freedom
- It is, nevertheless, necessary to seriously consider quantum effects (in addition to the finite number of components) when these systems are observed at extremely low temperatures

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7 OSS: è un modello quantistico ma possiamo usarlo classicamente perché a temperatura ambiente non ho più coerenza tra stati ⇒ spazio di Hilbert con semplici elementi fattorizzati ⇒ quindi l'interazione è pur avendo un'origine quantistica ho un modo di agire classico ⇒ ho fattorizzato lo spin

Mean Field theory and magnets

- Let's introduce interaction among spins. However, very few models of statistical mechanics have been solved exactly (the Ising model has been exactly solved in 1D and 2D); in most of the cases one has to rely on approximate methods.
- Among them, the mean-field approximation is one of the most widely used. The advantage of the mean-field theory is its simplicity and that it correctly predicts the qualitative features of a system in most cases; so in general it is the first instrument one resorts to when exploring new models
- As we have already seen with the van der Waals approach to a the fluid, the essence of the mean-field theory is the assumption of statistical independence of the local ordering (spins in the case of magnetic systems). The interaction terms in the Hamiltonian are replaced by an effective, "mean field" term. In this way, all the information on correlations in the fluctuations is lost

stesso peso statistico per ogni punto

- Therefore, the mean-field theory is usually inadequate in the critical regime. It usually gives wrong critical exponents, in particular at low spatial dimensions when the number of nearest neighbour is small.

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8 se i primi vicini sono pochi sono più rilevanti, ha meno senso una media

io ho sempre pensato che fosse $H = -\frac{1}{2} J \sum_{i} \sigma_i m$ che cos'è ?

- Let's consider the classical Ising Hamiltonian for a generic d-dimensional lattice of N spins:

$$H = -\tfrac{1}{2} J \sum_{\langle i,j \rangle_{n.n.}} \sigma_i \sigma_j - h \sum_{i=1}^{N} \sigma_i$$

- The magnetization, m, being: $m = \frac{1}{N} \left\langle \sum_{i=1}^{N} \sigma_i \right\rangle$

We have

$$\sigma_i \sigma_j = (\sigma_i - m + m)(\sigma_j - m + m) = -m^2 + m\sigma_i + m\sigma_j + \boxed{(\sigma_i - m)(\sigma_j - m)}$$

→ se mi focus sulla media ma do le fluttuazioni medie
↳ le trascuro

- The last term measures spin fluctuations; the mean field approximation neglects completely this term. The approximated Hamiltonian is

→ [illegible]

$$H_{MF} = -\tfrac{1}{2} J \sum_{\langle i,j \rangle_{n.n.}} \left[-m^2 + m\left(\sigma_i + \sigma_j\right) \right] - h \sum_{i=1}^{N} \sigma_i$$

- If n_{nn} is the coordination number of the lattice, i.e. the number of nearest neighbours, the H_{MF} turns out to be

$$H_{MF} = \frac{J N n_{nn}}{2} m^2 - (J n_{nn} m + h) \sum_{i=1}^{N} \sigma_i$$

H fattorizzato ⇒ p($\vec{\sigma}$) calcolabile

- With this approximation all the spins are decoupled form each other and thus it is easy to compute the partition function which turns out to be

$$Q_{MF} = \sum_{\{\sigma\}} e^{-\beta H_{MF}} = e^{-\beta J m^2 N n_{nn}/2} \left[\sum_{\sigma=\pm 1} e^{\beta (J n_{nn} m + h)\sigma} \right]^N = e^{-\beta J m^2 N n_{nn}/2} \left\{ 2\cosh\left[\beta \left(J n_{nn} m + h \right) \right] \right\}^N$$

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The Bragg-Williams equation

- The free energy per spin is given by $\frac{F}{N} = -\frac{k_B T}{N} \ln Q_{MF} = \frac{J m^2 n_{nn}}{2} - \frac{1}{\beta} \ln\left\{ 2\cosh\left[\beta \left(h + J n_{nn} m \right) \right] \right\}$

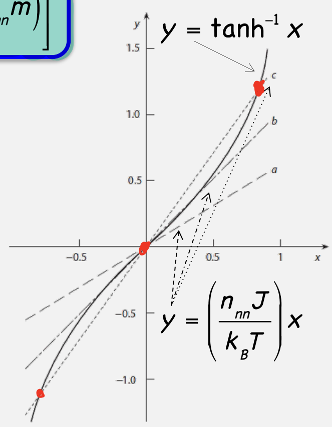
- The magnetization is given by $\boxed{m = -\frac{\partial (F/N)}{\partial h} = \tanh\left[\frac{1}{k_B T} \left(h + J n_{nn} m \right) \right]}$

which still the Bragg-Williams equation (1934/35).

- It is easier to discuss this equation in the form:

$$\tanh^{-1} m = \frac{h + n_{nn} J m}{k_B T}$$

which can be solved graphically.



- Consider the case h=0. The derivative of $\tanh^{-1}$ m assumes its minimum value in the origin, where it is equal to 1. Therefore, if $T > T_C = n_{nn} J / k_B$, the curve and the straight line have only one intersection, and there cannot be finite magnetization

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le soluzioni sono le intersezioni tra la $\tanh^{-1}$ e la retta

se $T > T_C = n_{nn} J / k_B$ ho solo $m = 0$ non posso avere magn spontanea

se $T < T_C$ ho anche $m = \pm m_0$

ma devi ancora minimizzare F ⇒ la soluzione fisica

- Instead, if $T < T_C$, there will be three solutions. Let call $\pm m_0$ the two solutions different from m=0. Which one is the "physical" solution? m=0, $m=m_0$ or $m=-m_0$?

- Let's go back to the free energy with h=0:

↳ l'equilibrio è a $\pm m_0$

$$\left.\frac{F}{N}\right|_{h=0} = \frac{Jm^2 n_{nn}}{2} - \frac{1}{\beta}\ln\left[2\cosh\left(\beta J n_{nn} m\right)\right]$$

usiamo sempre F perché a T costante

- when T $\rightarrow$0 F/N goes from a regime where it has only a minimum for m=0 to a regime where there are two equivalent minima for $m=\pm m_0 \neq 0$, as in figure

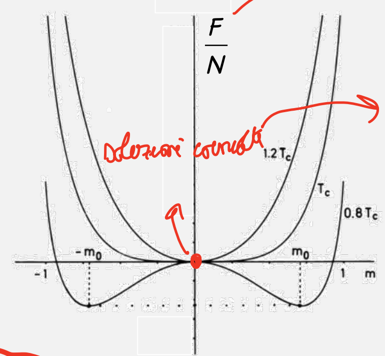
- Moreover

$$\left.\frac{\partial(F/N)}{\partial m}\right|_{h=0} = J n_{nn} m - J n_{nn}\tanh\left(\beta J n_{nn} m\right)$$

And from the Bragg-Williams equation:

$$\beta J n_{nn} m_0 = \tanh^{-1} m_0$$

$$\Rightarrow \boxed{\left.\frac{\partial(F/N)}{\partial m}\right|_{h=0;m=\pm m_0} = 0}$$



soluzioni coincidenti

T_c flesso tangente orizzontale

il sistema si mette per necessità in uno dei 2

- Thus $\pm m_0$ are the equilibrium values of the magnetization per spin; there is a perfect symmetry among $+m_0$ and $-m_0$ when h=0; to effectively realize a spontaneous magnetization with h=0 the system has to "choose" one of the two giving rise to a spontaneous symmetry breaking

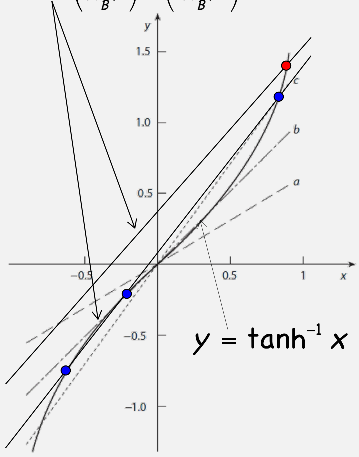
- Consider now the graphical solution of the Bragg-Williams equation for the case h>0 : we can have from only one (m_0>0) up to three solutions (m_1<0, m_2<0 and m_0>0), depending on the value of T and h

- In this case one can show that the free energy F is minimal for the solution with $m=m_0>0$. For h<0 the contrary is obtained

- Note that, independently from the value of h

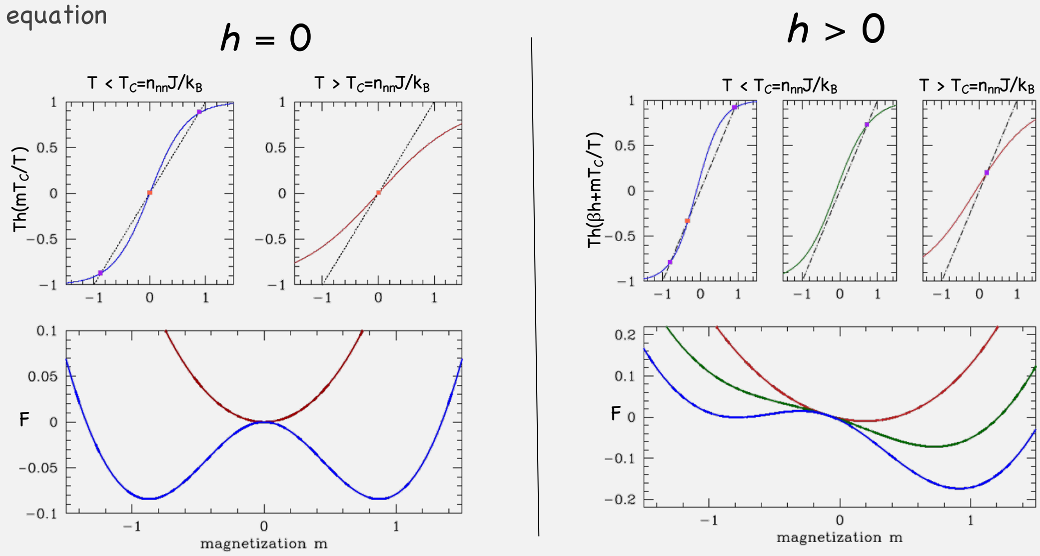
$$\lim_{T\to 0} m = \mathrm{sgn}(h)$$

$$y = \left(\frac{h}{k_B T}\right) + \left(\frac{n_{nn} J}{k_B T}\right) x$$



Solutions (Bragg-Williams equation)

- We can summarize in the following figure the graphical solutions of the Bragg-Williams equation



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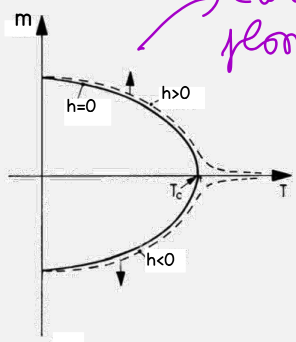
- Moreover, when $T \to T_C^-$ we have $m \ll 1$ and thus:

$$m = \tanh\left[m\frac{T_c}{T}\right] \underset{\text{Taylor}}{\approx} m\frac{T_c}{T} - \frac{m^3}{3}\underbrace{\left(\frac{T_c}{T}\right)^3}_{\approx 1} \Rightarrow \boxed{m \approx \sqrt{3\left(\frac{T_c - T}{T_c}\right)}} \quad \left(h = 0^+;\, T \to T_c^-\right)$$

- We obtain the following m-T phase diagram: (solid line: h=0; dashed line: h≠0)

c'entra con plommi?

- From the expression of H_{MF} (pag.9) with h=0



$$U = \left\langle H_{MF} \right\rangle_{h=0} = \frac{JNn_{nn}}{2}m^2 - Jn_{nn}m\left\langle \sum_{i=1}^{N} \sigma_i \right\rangle =$$

$$= \frac{JNn_{nn}}{2}m^2 - JNn_{nn}m^2 = -\frac{JNn_{nn}}{2}m^2$$

we can compute the specific heat which turns out to be

$$C_N = \left(\frac{\partial U}{\partial T}\right)_{N;h=0} = \begin{cases} 0 & T \geq T_c \\ -JNn_{nn}m\dfrac{\partial m}{\partial T} & T < T_c \end{cases}$$

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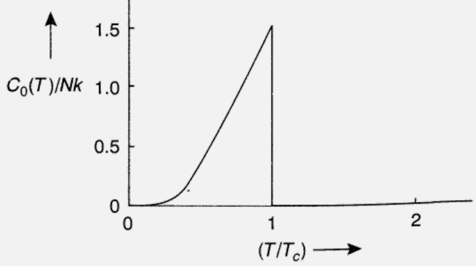
- Thus from $m \approx \sqrt{3\left(\frac{T_c - T}{T_c}\right)}$

$$m\frac{\partial m}{\partial T} \approx -\frac{3}{2T_c} \quad \Rightarrow \quad \lim_{T \to T_c^-} \frac{C_N}{N} = \frac{3}{2T_c} J n_{nn} = \frac{3k_B}{2} \qquad (h = 0)$$

sale e poi crolla a zero

- In conclusion:
  - for $T>T_C$ $m=0 \Rightarrow C_N=0$
  - for $T<T_C$ $C_N \neq 0$
  - For $T \to 0$ $m \to 1$ and $\partial m/\partial T \to 0$ $\Rightarrow C_N \to 0$



- If we would characterize the eventual presence of a "divergence" of the specific heat via a power law,

$$C = \left(\frac{\partial U}{\partial T}\right) \approx \begin{cases} (T - T_c)^{-\alpha} & (h \to 0;\ T \gtrsim T_c) \\ (T_c - T)^{-\alpha'} & (h \to 0;\ T \lesssim T_c) \end{cases}$$

in this case (Ising model, Mean Field approximation) we obtain $\alpha=\alpha'=0$, i.e. no divergence, only a gap.

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Critical exponents

le classi di universalità sono caratterizzate da anomalie critiche con scelte di potenza uguale

- In fact, a basic problem in the theory of phase transitions is to study the behavior of a given system in the neighborhood of its critical point.
- Experiments show that various physical quantities pertaining to the system possess singularities at the critical point.
- It is customary to express these singularities in terms of power laws characterized by a set of critical exponents which determine the qualitative nature of the critical behavior of the given system.
- To begin with, we identify an order parameter m, and the corresponding ordering field h, such that, in the limit $h \to 0$, m tends to a limiting value m_0 , with the property that $m_0=0$ for $T>T_C$ and $\neq 0$ for $T < T_c$
- For a magnetic system, the natural candidate for m is the magnetization, while for h is the external magnetic field; for a liquid-gas system, one may adopt the density differential $(\rho_l - \rho_c)$ and the pressure differential $(p-p_c)$ for h

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- The manner in which the order parameter m_0 tends to zero as $T \to T_C$ from below, defines the exponent β (Ising, Mean Field approximation we obtained: $\beta=1/2$)

$$m_0 \approx (T_c - T)^{\beta} \qquad (h \to 0;\ T \lesssim T_c)$$

- The manner in which the low-field (linear response) susceptibility χ diverges as $T \to T_C$ from above (below) defines the exponent γ (γ')

$$\chi = \left(\frac{\partial m}{\partial h}\right)_T \approx \begin{cases} (T - T_c)^{-\gamma} & (h \to 0;\ T \gtrsim T_c) \\ (T_c - T)^{-\gamma'} & (h \to 0;\ T \lesssim T_c) \end{cases}$$

In the gas-liquid transition, the role of χ is played by the isothermal compressibility.

- Next, we define an exponent δ by the eq. of state at $T=T_C$

$$m\big|_{T=T_c} \approx h^{1/\delta} \qquad (h \to 0;\ T = T_c)$$

magnetizz. critica rispetto al campo

- In the case of a gas-liquid system, δ is a measure of the degree of flatness of the critical isotherm at the critical point

$$\left|p - p_c\right|_{T=T_c} \approx \left|\rho - \rho_c\right|^{\delta} \qquad (p \to p_c;\ T = T_c)$$

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- Finally, we define exponents α and α' on the basis of the specific heat, C,

$$C = \left(\frac{\partial U}{\partial T}\right) \approx \begin{cases} (T - T_c)^{-\alpha} & (h \to 0;\ T \gtrsim T_c) \\ (T_c - T)^{-\alpha'} & (h \to 0;\ T \lesssim T_c) \end{cases}$$

- We have already determined this critical exponent for the Ising model solved in the Mean Field approximation $\alpha=\alpha'=0$; we now derive the other exponents.

- Let's start from the Bragg-Williams equation; for small h and $T \approx T_C$

$$m = \tanh\left[\frac{h}{k_B T} + m\frac{T_c}{T}\right] \approx \frac{h}{k_B T} + m\frac{T_c}{T} - \frac{1}{3}\left(\frac{h}{k_B T} + m\frac{T_c}{T}\right)^3$$

Which leads to the (approximate) magnetic equation of state:

$$\boxed{\frac{h}{k_B T} \approx m\frac{T - T_c}{T} + \frac{m^3}{3}}$$

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- Exactly at $T=T_C$ we find the critical isotherm:

$$\frac{h}{k_B T_C} \approx \frac{m^3}{3} \quad \Rightarrow \quad m \approx \left(\frac{3h}{k_B T_C}\right)^{\frac{1}{3}} \quad \Rightarrow \quad \boxed{\delta = 3}$$

- We now proceed to study the magnetic susceptibility of the system for $T \to T_C$ (thus m<<1) and h<<1 (linear response); we compute the isothermal magnetic susceptibility by differentiating the equation of state

$$\chi = \left(\frac{\partial m}{\partial h}\right)_T \quad \Rightarrow \quad \frac{1}{k_B T} \approx \chi \frac{T - T_C}{T} + \chi m^2 \qquad \chi \approx \frac{1/k_B T_C}{\frac{T - T_C}{T_C} + m^2}$$

- In the limit $h \to 0$ we can substitute the spontaneous magnetization m; for $T \to T_C^+$ we have m=0 thus

$$\chi \approx \frac{1}{k_B} \frac{1}{T - T_C}$$

- for $T \to T_C^-$ we can use $\quad m \approx \sqrt{3\left(\frac{T_C - T}{T_C}\right)} \quad \Rightarrow \quad \chi \approx \frac{1}{k_B} \frac{1}{2(T_C - T)}$

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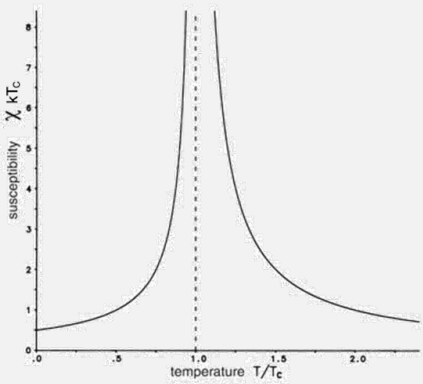
- The susceptibility is shown in the following figure:



The critical exponents γ and γ' turns out to be $\gamma=\gamma'=-1$

- The divergence of the magnetic susceptibility recall to us the divergence of the compressibility in the van der Waals fluid:

$$\chi = \left(\frac{\partial m}{\partial h}\right)_T = \frac{1}{N}\left(\frac{\partial M}{\partial h}\right)_T \qquad \kappa_T = -\frac{1}{V}\left(\frac{\partial V}{\partial p}\right)_{N,T}$$

- Both are susceptibilities which measure the variations of a generalized displacement due to the variations of the conjugate generalized force. To investigate more deeply this connection let's go back to the Bragg-Williams equation

$$m = \tanh\left[\frac{h}{k_B T} + m\frac{T_C}{T}\right]$$

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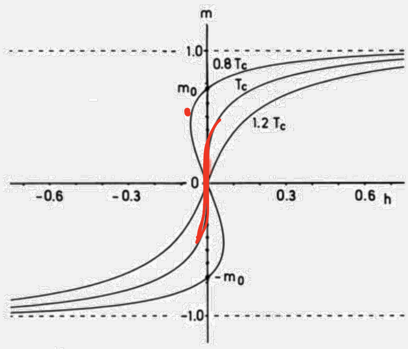
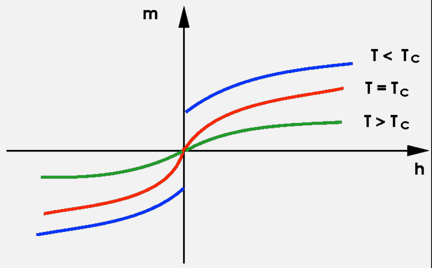
The thermodynamic surface

- In the m-h plane, the curves m(h) for different temperatures are shown here

These curves represent all the points (h,m) –event the unphysical ones– which mathematically solve the Bragg-Williams equation

- At $T \to T_C$ the susceptibility $\chi = \partial m / \partial h$ (for $h \to 0$) diverges, which means that $\partial h / \partial m \to 0$
- Therefore for $T<T_C$ there is a range in m in which $\partial h / \partial m < 0$ similarly to the van der Waals fluid where for $T<T_C$ we found an instable region characterized by $\partial p / \partial \rho < 0$ ($\partial p / \partial V > 0$)
- By excluding the unphysical points in the m-h plane we obtain a gap in the curves m(h) for $T<T_C$





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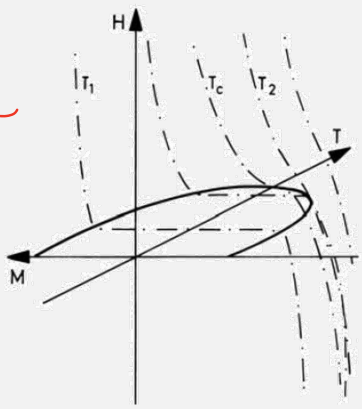
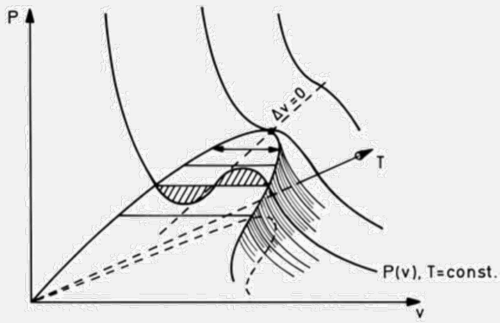
→ Transizioni di fase

- The thermodynamic surface of the Ising model solved within the Mean Field approximation is shown in the following figure; similarities with the critical point of the van der Waals fluid can be readily appreciated





- The differences among the two systems come from symmetry differences: in a magnet ↑or↓ are equivalent, in a fluid there is no liquid-gas symmetry

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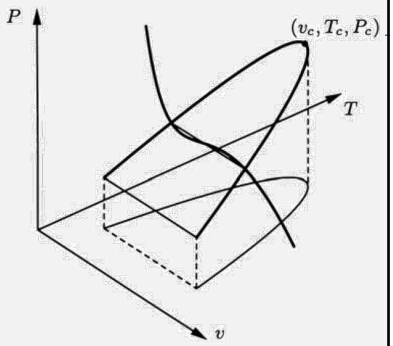
Van der Waals critical exponents

- Moreover, the van der Waals eq. of state has a linear term in the temperature which gives an inclination with respect to the V-T plane

$$\left[\tilde{p} + \frac{3}{\tilde{V}^2}\right]\left(3\tilde{V} - 1\right) = 8\tilde{T}$$

$$\left(\tilde{T} = \frac{T}{T_c}\,;\, \tilde{V} = \frac{V}{V_c}\,;\, \tilde{p} = \frac{p}{p_c}\right)$$



- In the close neighborhood of the critical point, from the van der Waals eq. of state one can compute the critical exponents. It turns out that (See Mean field theory / Critical exponent of a fluid system at: https://nptel.ac.in/courses/115/103/115103028/):

$$\beta = \frac{1}{2}\,;\, \delta = 3\,;\, \gamma = 1\,;\, \alpha = 0$$

- Exactly the same critical exponents found for the Ising model solved within the Mean field approximation

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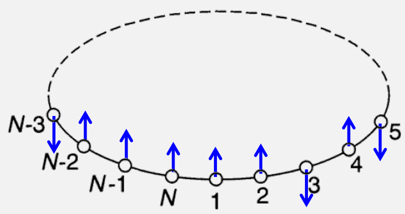
universalità ancora più potente a parità di dimensionalità d e di T_c

1D Ising model: the exact solution

- The 1D Ising model is one of very few models in statistical mechanics which are exactly solvable (2D Ising model is another –a true mathematical tour de force!– example)
- In a short paper published in 1925, Ising himself gave an exact solution to this problem in one dimension. Here we shall follow the transfer matrix method, first introduced by Kramers and Wannier in 1941.
- Three years later, in 1944, it became, through Onsager's intuition, the first method to treat successfully the field-free Ising model in two dimensions. In presence of an applied field there is (still) no exact solution in 2D to date; nor is there in 3D, with or without an applied field
- To apply this method, we use periodic boundary conditions, such that the N^{th} spin becomes a neighbor of the first.



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- This replacement eliminates the inconvenient end effects; it does not, however, alter the thermodynamic properties of the (infinitely long) chain. The important advantage of this replacement is that it enables us to write the Hamiltonian of the system in a symmetrical form

$$H = -J\sum_{i=1}^{N}\sigma_i\sigma_{i+1} - \tfrac{1}{2}h\sum_{i=1}^{N}\left(\sigma_i + \sigma_{i+1}\right)$$

because $\sigma_{N+1}=\sigma_1$

- The partition function of the system is then given by

$$Q_N(h,T) = \sum_{\sigma_1=\pm1}\cdots\sum_{\sigma_N=\pm1} e^{\beta\left[J\sum_{i=1}^{N}\sigma_i\sigma_{i+1}+\frac{1}{2}h\sum_{i=1}^{N}(\sigma_i+\sigma_{i+1})\right]} =$$

$$= \sum_{\sigma_1=\pm1}\cdots\sum_{\sigma_N=\pm1}\left\langle\sigma_1\middle|\mathrm{P}\middle|\sigma_2\right\rangle\left\langle\sigma_2\middle|\mathrm{P}\middle|\sigma_3\right\rangle\cdots\left\langle\sigma_{N-1}\middle|\mathrm{P}\middle|\sigma_N\right\rangle\left\langle\sigma_N\middle|\mathrm{P}\middle|\sigma_1\right\rangle$$

→ sono completezze

Where **P** denotes an operator with matrix elements

$$\left\langle\sigma_i\middle|\mathrm{P}\middle|\sigma_{i+1}\right\rangle = e^{\beta\left[J\sigma_i\sigma_{i+1}+\frac{1}{2}h(\sigma_i+\sigma_{i+1})\right]} \quad\Rightarrow (\mathrm{P}) = \begin{pmatrix} \langle\uparrow|\mathrm{P}|\uparrow\rangle & \langle\uparrow|\mathrm{P}|\downarrow\rangle \\ \langle\downarrow|\mathrm{P}|\uparrow\rangle & \langle\downarrow|\mathrm{P}|\downarrow\rangle \end{pmatrix} = \begin{pmatrix} e^{\beta[J+h]} & e^{-\beta[J]} \\ e^{-\beta[J]} & e^{\beta[J-h]} \end{pmatrix}$$

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- According to the rules of matrix algebra, the summations over the various σ_i in the equation for $Q_N(h,T)$ lead to the simple result

$$Q_N(h,T) = \sum_{\sigma_1=\pm1}\left\langle\sigma_1\middle|\mathrm{P}^N\middle|\sigma_1\right\rangle = Tr\left(\mathrm{P}^N\right) = \lambda_1^N + \lambda_2^N$$

where λ_1 and λ_2 are the eigenvalues of the matrix **P**

- These eigenvalues are given by the equation

$$\det\left(\mathrm{P}-\lambda\mathbf{I}\right) = \det\begin{pmatrix} e^{\beta[J+h]}-\lambda & e^{-\beta[J]} \\ e^{-\beta[J]} & e^{\beta[J-h]}-\lambda \end{pmatrix} = 0$$

- That is by

$$\lambda^2 - 2\lambda e^{\beta J}\cosh\left(\beta h\right) + 2\sinh\left(2\beta J\right) = 0$$

- One readily obtains

$$\boxed{\lambda_{1,2} = e^{\beta J}\cosh\left(\beta h\right) \pm \sqrt{e^{-2\beta J} + e^{2\beta J}\sinh^2\left(\beta h\right)}}$$

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- Quite generally, $\lambda_1 > \lambda_2$; so, $(\lambda_2/\lambda_1)^N \to 0$ as $N \to \infty$

- It is only the larger eigenvalue, λ_1 ,that determines the major physical properties of the system in the thermodynamic limit:

$$Q_N(h,T) = \lambda_1^N + \lambda_2^N \quad \Rightarrow \quad A(h,T) = -k_B T \ln Q_N(h,T) \approx -k_B TN \ln \lambda_1 =$$

$$= -k_B TN \ln\left[e^{\beta J}\cosh(\beta h) + \sqrt{e^{-2\beta J} + e^{2\beta J}\sinh^2(\beta h)}\right]$$

$$\Rightarrow \boxed{A(h,T) = -NJ - k_B TN \ln\left[\cosh(\beta h) + \sqrt{e^{-4\beta J} + \sinh^2(\beta h)}\right]}$$

- The various other properties of the system follow readily from the Helmholtz free energy. For example, it is extremely important to consider the magnetization per spin

$$m = \frac{\langle M \rangle}{N} = -\left(\frac{\partial A/N}{\partial h}\right)_T = \frac{\partial}{\partial h}\left\{J + k_B T \ln\left[\cosh(\beta h) + \sqrt{e^{-4\beta J} + \sinh^2(\beta h)}\right]\right\}$$

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perché ho dimenticato le fluttuazione
e questi non posso avere contributi che "medono" a β

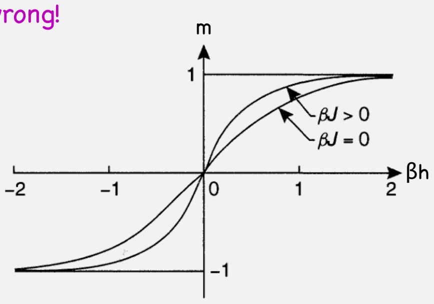
$\sum_n \mapsto \int$

We found that

$$m = \frac{\dfrac{\sinh(\beta h)\cosh(\beta h)}{\sqrt{e^{-4\beta J} + \sinh^2(\beta h)}} + \sinh(\beta h)}{\cosh(\beta h) + \sqrt{e^{-4\beta J} + \sinh^2(\beta h)}} = \boxed{\frac{\sinh(\beta h)}{\sqrt{e^{-4\beta J} + \sinh^2(\beta h)}}}$$

- We note that, as $h \to 0$, $m \to 0$ for all finite temperatures. This rules out the possibility of spontaneous magnetization, and hence of a phase transition, at any finite temperature T. Mean Filed approximation for the 1D Ising model is wrong!

- Of course, at T = 0, m (for any value of h) is equal to the saturation value 1, which implies perfect order in the system. This means that there is, after all, a phase transition at a critical temperature T_C, which coincides with absolute zero!



- In figure the paramagnetic model result (no interaction: J=0) is also shown: $m = \tanh(\beta h)$

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- The low-field magnetic susceptibility of the system is given by the initial slope of the magnetization curve; one obtains

$$\chi = \lim_{h\to 0}\left(\frac{\partial M}{\partial h}\right) = \lim_{h\to 0}\frac{\partial}{\partial h}\frac{N\sinh(\beta h)}{\sqrt{e^{-4\beta J}+\sinh^2(\beta h)}} =$$

$$= \lim_{h\to 0} N \frac{\beta\cosh(\beta h)\sqrt{e^{-4\beta J}+\sinh^2(\beta h)} - \sinh(\beta h)\frac{1}{2}\frac{2\beta\sinh(\beta h)\cosh(\beta h)}{\sqrt{e^{-4\beta J}+\sinh^2(\beta h)}}}{\left[e^{-4\beta J}+\sinh^2(\beta h)\right]} =$$

$$= \lim_{h\to 0}\beta N\frac{\cosh(\beta h)\left[e^{-4\beta J}\cancel{+\sinh^2(\beta h)}\right]\cancel{-\sinh^2(\beta h)\cosh(\beta h)}}{\left[e^{-4\beta J}+\sinh^2(\beta h)\right]^{3/2}} =$$

$$\Rightarrow \chi = \lim_{h\to 0}\beta N\frac{\cosh(\beta h)e^{-4\beta J}}{\left[e^{-4\beta J}+\sinh^2(\beta h)\right]^{\frac{3}{2}}} = \frac{N}{k_B T}e^{2J/k_BT}$$

which diverges as T→0

- For T→∞ the magnetic susceptibility decays with the Curie's law for paramagnets.

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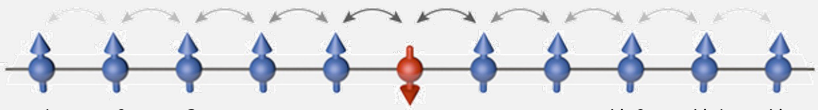
1D Ising model: correlations

niente pbc

- We consider now a 1D Ising model with an open chain lattice:



1 2 3 ... ... N-2 N-1 N

- We proceed to calculate the correlation function of two spins σ_i and σ_j for h=0, which is defined as (with i≤j≤N) :

$$\boxed{G_{ij} = \langle\sigma_i\sigma_j\rangle - \langle\sigma_i\rangle\langle\sigma_j\rangle}$$

perché per h=0 $\langle\sigma_i\rangle=0$

perché $\langle\sigma_i\rangle \propto m$

mi serve $Q_N(T)$

risulta meglio

$$G_{ij} = \frac{1}{Q_N(T)}\sum_{\sigma_1=\pm1}\cdots\sum_{\sigma_N=\pm1}\sigma_i\sigma_j e^{\beta J\sum_{i=1}^{N-1}\sigma_i\sigma_{i+1}} - \cancel{\langle\sigma_i\rangle\langle\sigma_j\rangle}\to 0$$

- We can write the partition function in a different way:

$$Q_N(T) = \sum_{\sigma_1=\pm1}\cdots\sum_{\sigma_N=\pm1}e^{\beta J\sum_{i=1}^{N-1}\sigma_i\sigma_{i+1}} = \Big|_{(\beta J=K_i)\forall i}\sum_{\sigma_1=\pm1}\cdots\sum_{\sigma_N=\pm1}e^{\sum_{i=1}^{N-1}K_i\sigma_i\sigma_{i+1}}$$

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per fare i calcoli serve $\beta J = k_i \; \forall i$

altro modo: $\langle\sigma_i\rangle = \sum\sum\sigma_i e^{-\beta H} = 0$ f. dispari COSA

Lezione

- with $K_i=\beta J$ where J is the exchange interaction between the i^{th} spin and the $(i+1)^{th}$ spin along the chain. Of course, at the end of our calculation we shall take the limit $K_1 = K_2 = \ldots = K_{N-1} = \beta J$ and $N\to\infty$

- Carrying out the summation only over the spin configurations σ_N, we get

$$Q_N(T) = \sum_{\sigma_1=\pm1}\cdots\sum_{\sigma_{N-1}=\pm1} e^{\sum_{i=1}^{N-2} K_i\sigma_i\sigma_{i+1}}\left(e^{K_{N-1}\sigma_{N-1}} + e^{-K_{N-1}\sigma_{N-1}}\right) = \cdots$$

- Regardless of the value of σ_{N-1}, the factor in round brackets turns out to be always equal to $2\cosh(K_{N-1})$. Thus we can write

$$Q_N(T) = Q_N(T,K_1,\cdots,K_{N-1}) = \left[2\cosh\left(K_{N-1}\right)\right]Q_{N-1}(T,K_1,\cdots,K_{N-2})$$

- Iterating this summation successively over the spins, we finally get (see supplementary material):

$$Q_N(T) = \sum_{\sigma_1=\pm1}\prod_{i=1}^{N-1}2\cosh\left(K_i\right) = 2\prod_{i=1}^{N-1}2\cosh\left(K_i\right)$$

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- For $r>0$ and $j=(i+r)\leq N$, the two-spin correlation function can be written as

$$G_{i,i+r} = \frac{1}{Q_N(T)}\sum_{\sigma_1=\pm1}\cdots\sum_{\sigma_N=\pm1}\sigma_i\sigma_{i+r}e^{\sum_{i=1}^{N-1}K_i\sigma_i\sigma_{i+1}}$$

- Now we use that [$\sigma_l^2=1$ $\forall l$] to obtain

→ uguale a quando usavi la P-matrix

$$G_{i,i+r} = \frac{1}{Q_N(T)}\sum_{\sigma_1=\pm1}\cdots\sum_{\sigma_N=\pm1}\underbrace{\left(\sigma_i\sigma_{i+1}\right)}_{1}\underbrace{\left(\sigma_{i+1}\sigma_{i+2}\right)}_{1}\cdots\underbrace{\left(\sigma_{i+r-2}\sigma_{i+r-1}\right)}_{1}\underbrace{\left(\sigma_{i+r-1}\sigma_{i+r}\right)}_{1}e^{\sum_{i=1}^{N-1}K_i\sigma_i\sigma_{i+1}}$$

- Note that, one can rewrite this expression for the two-spin correlation function in the form

$$G_{i,i+r} = \frac{1}{Q_N(T,K_1,\cdots,K_{N-1})}\frac{\partial^r Q_N(T,K_1,\cdots,K_{N-1})}{\partial K_{i+r-1}\cdots\partial K_i}$$

Nota $G_{i,j}$ come funzione di Green

evaluated at $K_1 = K_2 = \ldots = K_{N-1} = \beta J$ after differentiation.

- Substituting the obtained expression for $Q_N(T)$ we get

$$G_{i,i+r} = \frac{1}{2^N\prod_{i=1}^{N-1}\cosh\left(K_i\right)}\left[2^{N-l}\prod_{j\notin[i,i+r]}\cosh\left(K_j\right)\right]\left[2^l\prod_{j\in[i,i+r]}\sinh\left(K_j\right)\right] = \left(\tanh\beta J\right)^r$$

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The correlation length

- An expression for the correlation length can be extracted from the exact expression for the two-spins correlation function by re-expressing it as an exponentially decaying function of the separation r

$$G_{i,i+r} = \left(\tanh \beta J\right)^r = e^{\ln\left[\left(\tanh \beta J\right)^r\right]} = e^{r\left[\ln\left(\tanh \beta J\right)\right]} = e^{-r/\xi}$$

where the correlation length ξ is given by $\xi = -\left\{\ln\left[\tanh\left(J/k_B T\right)\right]\right\}^{-1}$ ricordati che sei partito a primi vicini

- Given that $\tanh(J/k_B T) \leq 1$, note that $\xi \geq 0$ for all T

- Recall that in the case of the 1D nearest-neighbour Ising model

(a) m=0 for all T>0, but m=±1 at T=0

(b) $\chi \to \infty$ as $T \to 0$

(c) ξ is finite for all T>0, but $\xi \to \infty$ as $T \to 0$ a T=0 ho correlazione e quindi magnetizzazione spontanea

i.e. there is no long-range correlation between the spins at any T≠0

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The critical exponent ν

- It can also be shown through exact calculations that for the same model in 2D

(a) $T_C>0$; m=0 for all $T>T_C$ if h=0; m>0 at $T<T_C$

(b) $\chi \to \infty$ as $T \to T_C$

(c) $\xi \to \infty$ as $T \to T_C$

and the correlation length ξ exhibits a power-law divergence at T_C in 2D in contrast to its exponential divergence in 1D.

- One can introduce a new critical exponents, ν, in order to describe the critical behavior of the correlation length:

$$\xi \approx \begin{cases} \left(T - T_c\right)^{\nu} & \left(h \to 0;\ T > T_c\right) \\ \left(T_c - T\right)^{\nu'} & \left(h \to 0;\ T < T_c\right) \end{cases}$$

- In the next we shall present a physical argument to explain why long-range ferromagnetic ordering happens at non-vanishing temperatures in 2D but not in 1D

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Energy vs Entropy

- The nature of the state of thermal equilibrium is determined by the minimum of $F = E - TS$, which is crucially dependent on the competing effects of the energy and the entropy
- Energy is lowered if the system exhibits "order" whereas the gain of entropy usually favours "disorder"
- Clearly, entropy must be dominating over energy in the one-dimensional Ising model at all $T > 0$, whereas the energy must dominate over entropy in the range $0 < T < T_C$ in the case of the two-dimensional Ising model.
- The reason for this dimensionality dependence was explained by Peierls (1936) and his arguments were made more rigorous later by Griffiths (1964, 1972; see supplementary material!). In the next slides we present the argument in 1D to explain why the entropy dominates over energy at all T>0.

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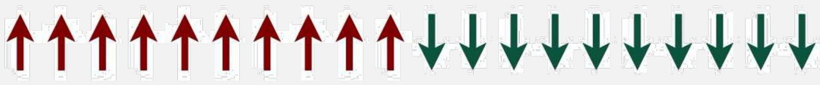
1D Ising model: domain walls

- Consider a open chain consisting of N Ising spins. At $T = 0$ this system with $h=0$ has two ground states, [↑↑↑↑…↑] and [↓↓↓↓ … ↓]. The ground state energy is given by $E_0=-(N-1)J$
- To choose between these ground states, we can specify a boundary condition at the ends of our one-dimensional chain, where we demand that the spins are up. Equivalently, we can apply a magnetic field h of order 1/N, which vanishes in the thermodynamic limit, but which at zero temperature will select the "all up" ground state.
- The lowest-energy excitation of this system correspond to a single interface, which is a sharp domain wall separating the "all-up" region on one side from the "all-down" region on the other side of it



- in 1D domain walls live on individual links

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M DOMINI grandi x ?

- The energy difference between this excited state and the ground state is 2J:

$$\cdots \uparrow\uparrow\uparrow\downarrow\downarrow\downarrow \cdots \qquad \left(\Delta J_{-J\to+J} = 2J\right)$$

-J -J +J -J -J

- For a system with M = xN domain walls, x representing their concentration and N the number of lattice sites, the free energy difference is

$$\Delta A = \Delta E - TS = 2JM - k_B T \ln \frac{N!}{M!(N-M)!} \approx \leftarrow \text{Stirling}$$

(see supplementary material) $\quad \cdots = N\left\{2Jx + k_B T\left[x \ln x + (1-x)\ln(1-x)\right]\right\}$

- Minimizing the free energy difference with respect to x, one finds

$$\frac{\partial(\Delta A/N)}{\partial x} = 2J + k_B T\left[\ln x - \ln(1-x)\right] = 0 \quad \Rightarrow \quad x = \frac{1}{1 + e^{2J/k_B T}}$$

- So the equilibrium concentration of domain walls is finite, meaning there can be no long-ranged spin order. In 1D, entropy wins and there is always a thermodynamically large number of domain walls in equilibrium

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perché se ho una correlazione non nulla ho $\langle m \rangle = 0 \Rightarrow$ VINCE ENTROPIA

$$\cdots \uparrow\uparrow\uparrow\downarrow\downarrow\downarrow \cdots$$

-J -J +J -J -J

- We can obtain the same conclusion noting that since the interface could occur at any of the N-1 positions, the corresponding entropy is $k_B \ln(N-1)$.
  Therefore, the change in the free energy caused by the creation of such a single interface is

$$\Delta A = 2J - k_B T \ln(N-1)$$

- Since this energy is independent of N but the entropy increases with N, the entropy dominates over energy in the thermodynamic limit, no matter however small the temperature may be

- Thus, in 1D, the system can lower the free energy by creating an interface at any temperature T > 0

- Infact, the free energy can be lowered further by splitting each domain into two parts and this process can be continued. In other words, in 1D, the long-range order is unstable with respect to thermal fluctuations

in 1D VINCE L'ENTROPIA SEMPRE → SIST. DISORDINATO

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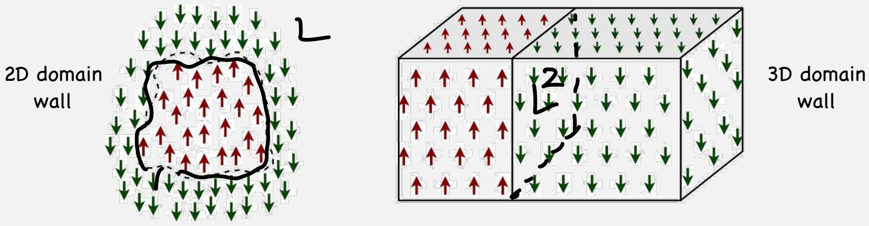
per semplicità mi riduco a ipersuperfici di separazioni brutte

Ising Ferromagnetism for d>1

- Consider next an Ising domain wall in d dimensions. Let the linear dimension of the system be La, where L is a real number and a is the lattice constant.



- Then the energy of a single domain wall which partitions the entire system is $2JL^{d-1}$
- The domain wall entropy is difficult to compute, because the wall can fluctuate significantly, but for a single domain wall we have $S \gtrsim k_B \ln L$
- Thus, the free energy $A \approx (2JL^{d-1}) - (k_B T \ln L)$ should be dominated by the energy term if $d \geqslant 2$, suggesting that the system may be ordered. This is different from the situation in one dimension. In one dimension, if the density of the partition points is nonzero, we have positive and negative regions. The lengths of each region can be changed without expenditure of energy.

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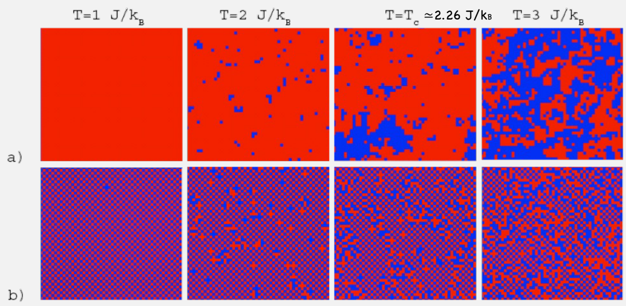
- In two dimensions, although the density of partition lines is nonzero, the negative regions cannot increase at low temperature because expansion requires longer boundary lines and hence more energy. The result is similar in three dimensions, where partition lines become partition surfaces. At low temperatures, except for some small regions, all the spins will point to the same direction.
- Lars Onsager famously solved the 2D Ising model (for h=0) exactly in 1944. His solution provided a closed-form expression for the free energy in the thermodynamic limit, marking a major milestone in statistical mechanics:

$$T_c = \frac{2J}{k_B \sinh^{-1} 1}$$

$$M \underset{T<T_c}{=} N \frac{\cosh^2(2J/k_BT)}{\sinh^4(2J/k_BT)}\left[\sinh^2(2J/k_BT) - 1\right]^{\frac{1}{8}}$$

$$\frac{M}{N} \underset{T \approx T_c}{\approx} (T - T_c)^{\frac{1}{8}}$$



Output of MC simulations of the 2D-Ising model. Each red (blue) square represents an up (down) spin.
a) ferromagnetic case, J > 0;
b) anti-ferromagnetic case, J < 0.

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a $T = T_c$ $\langle m \rangle = 0$ ma fluttuazioni a qualunque scala

↳ vedo domini a qualunque scala

Lecture 3: Suggested books

- L. Peliti, "Appunti di meccanica statistica", Bollati Boringhieri
- R. Piazza "Note di Fisica Statistica" Springer
- R. K. Pathria, "Statistical mechanics", II ed., Oxford
- Shang-Keng Ma, "Statistical mechanics", World Scientific

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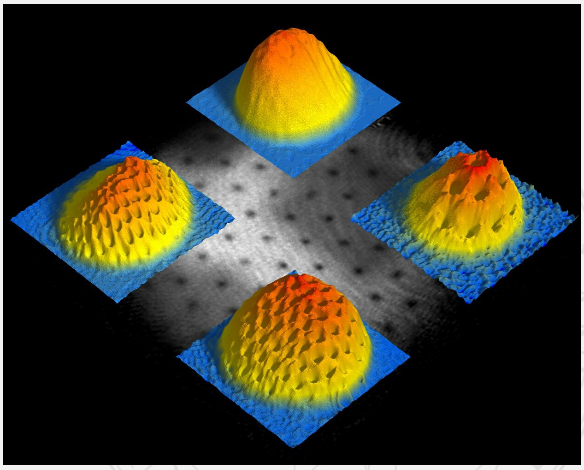
UNIVERSITÀ DEGLI STUDI DI MILANO

Advanced Statistical Physics

Lecture 3

Supplementary material



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Partition function of the 1D Ising open chain:

$$Q_N(T) = \sum_{\sigma_1=\pm1} \cdots \sum_{\sigma_N=\pm1} e^{\beta J \sum_{i=1}^{N-1} \sigma_i \sigma_{i+1}} = \Big|_{(\beta J = K_i)\forall i} \sum_{\sigma_1=\pm1} \cdots \sum_{\sigma_N=\pm1} e^{\sum_{i=1}^{N-1} K_i \sigma_i \sigma_{i+1}}$$

$$Q_N(T) = \sum_{\sigma_1=\pm1} \cdots \sum_{\sigma_{N-1}=\pm1} e^{\sum_{i=1}^{N-2} K_i \sigma_i \sigma_{i+1}} \left(e^{K_{N-1}\sigma_{N-1}} + e^{-K_{N-1}\sigma_{N-1}} \right) = \cdots$$

$$\left(e^{K_{N-1}\sigma_{N-1}} + e^{-K_{N-1}\sigma_{N-1}} \right) = 2\cosh\left(K_{N-1}\sigma_{N-1}\right) = 2\cosh\left(K_{N-1}\right)$$

$$Q_N(T) = Q_N(T, K_1, \cdots, K_{N-1}) = \left[2\cosh\left(K_{N-1}\right)\right] Q_{N-1}(T, K_1, \cdots, K_{N-2})$$

$$Q_N(T, K_1, \cdots, K_{N-1}) = \left[2\cosh\left(K_{N-1}\right)\right]\left[2\cosh\left(K_{N-2}\right)\right] Q_{N-2}(T, K_1, \cdots, K_{N-3}) =$$

$$Q_N(T, K_1, \cdots, K_{N-1}) = \left[2\cosh\left(K_{N-1}\right)\right] \cdots \left[2\cosh\left(K_2\right)\right] Q_2(T, K_1) =$$

$$Q_2(T, K_1, K_2) = \sum_{\sigma_1=\pm1} \sum_{\sigma_2=\pm1} e^{K_1 \sigma_1 \sigma_2} \Rightarrow Q_2(T, K_1) = \sum_{\sigma_1=\pm1}$$

$$Q_N(T) = \sum_{\sigma_1=\pm1} \prod_{i=1}^{N-1} 2\cosh\left(K_i\right) = 2\prod_{i=1}^{N-1} 2\cosh\left(K_i\right)$$

c.v.d.

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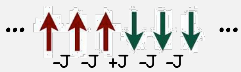
Free energy for a domain wall in 1D:



$$F = E - TS = 2JM - k_B T \ln \frac{N!}{M!(N-M)!} =$$

$$\approx 2JM - k_B T \left[N \ln N - M \ln M - (N-M)\ln(N-M) \right] =$$

$$= 2JM - k_B T \left\{ N \ln N - M \ln M - N(1-x) \ln\left[N(1-x)\right] \right\} =$$

$$= 2JM - k_B T \left\{ N \ln N - M \ln M - N(1-x)\left[\ln N + \ln(1-x)\right] \right\} =$$

$$= 2JM - k_B T N \left\{ -x \ln M + x \ln N - (1-x)\ln(1-x) \right\} =$$

$$= 2JNx + k_B T N \left\{ x \ln x + (1-x)\ln(1-x) \right\} =$$

$$= N\left\{ 2Jx + k_B T \left[x \ln x + \left(1-x\right)\ln\left(1-x\right) \right] \right\}$$

c.v.d.

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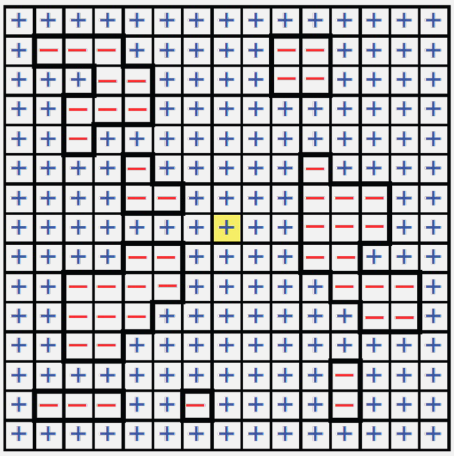
Existence of Ising Ferromagnetism in 2D

- One can repeat the above argument more rigorously for the two dimensional case. Consider the Ising model, in zero magnetic field, on a NxN square lattice, with N→∞ in the thermodynamic limit.
- To prove the existence of ferromagnetism is to prove that in zero external magnetic field and at nonzero temperatures, the average value of the spin is nonzero
- In Figure some values of the spins (+1 or -1, abbreviated as +, -) are shown. There exists a partition segment (1D domain wall) between every pair of neighbouring spins with opposite signs. These segments can be joined to form partition lines (2D domain walls), dividing the whole lattice into regions.
- The length of the partition line is determined by the number of segments in the line.



- The total magnetization is the area of positive regions minus that of negative regions.
- Obviously, to create partition lines, energy must be spent. At T = 0 all the spins are in the same direction (say positive), and there is no partition line. When the temperature is increased to T, negative regions will appear. If the perimeter of a certain negative region is L, the energy, with respect to the ground state energy, is 2JL because the energy of each partition point is 2J
- Assuming that N is odd, in the middle point of our 2D lattice we have a spin. Take this spin as σ_0 . Let the probabilities that σ_0 is + 1 or -1 be p_+ and p_- . Then

$$\langle \sigma_0 \rangle = p_+ - p_-$$

- Now we have to prove that if T is sufficiently small, $\langle\sigma_0\rangle \neq 0$
- Let all the spins at the boundary of the square lattice be + 1 and let us focus our attention on the spin at the origin σ_0

- Even in absence of an external magnetic field, the fixed "+" signs on the boundary tend to make the lattice sites near them be positive with higher probability.
- When the temperature is high this effect is quickly dissipated, but for low T it is possible that the effect will travel a considerable distance inward. We will show that for sufficiently low T p_- is less than ½ by an amount which is independent of the lattice size
- Recall that the probability for a given configuration $\sigma=(\sigma_1,\ldots,\sigma_N)$ is given by

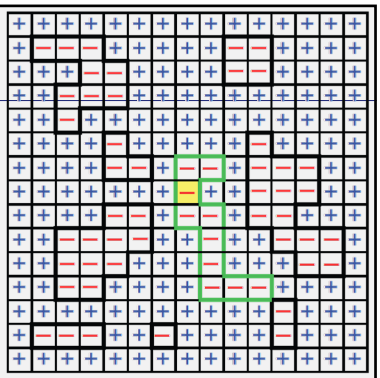
$$p(\sigma) = \frac{e^{-\beta H(\sigma)}}{Q}$$

- where $H(\sigma)$ is the energy of the particular configuration and Q is the partition function

$$Q = \sum_{\sigma\in\Gamma} e^{-\beta H(\sigma)}$$

- where Γ is the set of all configurations which are positive on the boundary

- Now we distinguish the configurations $\sigma\in\Gamma$ into two sets: the set Γ^+ contains all configurations in which σ_0 is equal to +1, and the set Γ^- contains all the others in which σ_0 is equal to -1. $\Gamma = \Gamma^+ \cup \Gamma^-$



- Then

$$p_- = \frac{1}{Q}\sum_{\sigma\in\Gamma^-} e^{-\beta H(\sigma)}$$

- If σ_0 is -1, then it must be surrounded by one loop or three loops or five loops.., of closed partition lines.
- The number of loops must be odd. (If it is surrounded by 2 loops or 4 or 6… loops, σ_0 must be +1. If there is no loop surrounding it, naturally it is +1)
- Suppose now we draw a partition line Υ which includes σ_0 and say that its length is $L(\Upsilon)$. Let's consider the subset $\Omega^-\subset\Gamma^-$ of configurations having Υ as the innermost partition line.

Then

$$p(\Omega^-) = \frac{1}{Q}\sum_{\sigma\in\Omega^-} e^{-\beta H(\sigma)} = \frac{e^{-2\beta J L(\gamma)}}{Q}\sum_{\sigma\in\Omega^-} e^{\beta\frac{J}{2}\sum_{i,j(\notin\gamma)}\sigma_i\sigma_j}$$

- Given σ∈Ω^-, if we change σ_0 and all the spins within ϒ to +1, we get one loop less and this is a configuration for σ_0= +1. We will call σ' such new configuration; obviously σ'∈Γ^+
- For a fixed ϒ, the map σ→σ' is one to one. We shall let Ω^+ denote the image of Ω^- under this mapping.

One easily sees that

$$\sum_{i,j(\notin\gamma)} \sigma_i \sigma_j = \sum_{i,j} \sigma'_i \sigma'_j - L(\gamma) \quad \Rightarrow \quad \boxed{\sum_{i,j(\notin\gamma)} \sigma_i \sigma_j < \sum_{i,j} \sigma'_i \sigma'_j}$$

- Plugging this inequality into the previous probability, we have

$$p(\Omega^-) < \frac{e^{-2\beta J L(\gamma)}}{Q} \sum_{\sigma'\in\Omega^+} e^{\beta\frac{J}{2}\sum_{i,j}\sigma'_i\sigma'_j} = e^{-2\beta J L(\gamma)} \frac{1}{Q} \sum_{\sigma'\in\Omega^+} e^{-\beta H(\sigma')}$$

- We have also used the fact that σ→σ' is one to one, so that the sum over Ω^- can be replaced by the sum over Ω^+

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- But now, since $e^{-\beta H}>0$ for all configurations σ, we can replace the sum over Ω^+ by a sum over all configurations. Thus

$$p(\Omega^-) < e^{-2\beta J L(\gamma)} \frac{1}{Q} \sum_{\sigma\in\Gamma} e^{-\beta H(\sigma)} = e^{-2\beta J L(\gamma)}$$

- Now consider the set G of all the partition lines which surround the origin of the lattice

$$p_- = \sum_{\gamma\in G} p(\Omega^-) < \sum_{\gamma\in G} e^{-2\beta J L(\gamma)} = \sum_{L=4}^{\infty} g(L)\, e^{-2\beta J L}$$

- where g(L) represents the number of configurations with length L for the innermost loop (Note also that here the symmetry of our reasoning among p_- and p_+ breaks since you cannot write p_+ only as a sum on partition lines, e.g. you can have configurations without any partition line surrounding the origin which contribute to p_+).
- g(L) naturally depends on the positions of the other partition lines. We cannot draw a loop intersecting the other loops. But if we neglect this restriction and count all the configurations looping σ_0 once, then we over-estimate g(L)
- The factor g(L) in the previous formula will be calculated neglecting the existence of the outer loops.

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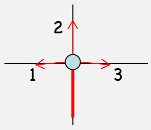
- Starting from any point, there are 3 ways of drawing the next steps, i.e. except for going back on the previous step, the remaining 3 directions can be chosen.



- To draw L steps we have $4 \times 3^{L-1}$ ways. The 4 comes from the first step, when all the four directions are permissible.
- We require L to return to the starting position. So the total number is less than $4 \times 3^{L-1}$. In addition we can start from any point on the loop, clockwise or anticlockwise. Therefore we should divide $4 \times 3^{L-1}$ by 2L. We can write

$$g(L) < \frac{4}{2L} 3^{L-1} \left(\frac{L}{4}\right)^2$$

- The factor $(L/4)^2$ is just the largest area that can be enclosed by the partition line, i.e. a square with side L/4. Because σ_0 can be any point within the loop, it is obvious that g(L) must contain this area factor.
- Substituting this inequality, we get: $P_- < \sum_{L=4}^{\infty} \frac{L}{8} 3^{L-1} e^{-2\beta J L}$

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- Notice that the shortest loop is L = 4 and L must be even. We add the odd terms and get

$$P_- < \sum_{L=4}^{\infty} \frac{L}{8} 3^{L-1} e^{-2\beta J L} = \frac{1}{24} \sum_{L=4}^{\infty} L \left(3e^{-2\beta J}\right)^L < \frac{1}{24} \sum_{L=1}^{\infty} L \left(3e^{-2\beta J}\right)^L$$

- This series is easily computed. Recall that: $\frac{1}{1-x} = 1 + x + x^2 + \cdots = \sum_{n=0}^{\infty} x^n \quad if\ |x| < 1$
- Hence, by differentiating and multiplying by x: $\frac{x}{(1-x)^2} = x(1 + 2x + 3x^2 + \cdots) = \sum_{n=1}^{\infty} n x^n$
- Thus, letting $x=3e^{-2\beta J}$, we have $P_- < \frac{1}{24} \frac{3e^{-2\beta J}}{\left(1-3e^{-2\beta J}\right)^2}$
- The conclusion is clear: by taking β sufficiently large or T sufficiently low, the right-hand side of this inequality: $\boxed{P_- < \frac{1}{2} \frac{e^{-2\beta J}}{4\left(1-3e^{-2\beta J}\right)^2}}$

can be made arbitrarily small, in a way which is independent of the size of the lattice. Thus spontaneous magnetization is guaranteed at some low temperature in 2D!

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