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On a mean-field theory of the Ising ferromagnet

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Abstract

A new mean-field approach to the Ising model is presented, with the aim of attaining an insight into the nature of the ferromagnetic phase transition.

The Ising model was shown to exhibit no transition in one dimension,[1] while it has ferromagnetically ordered phases in two and three dimensions, below a critical temperature. The model has been solved exactly in two dimensions[2], after the critical temperature had previously been located.[3] An exact solution is still lacking in three dimensions, though a great deal of results are known.[4] Approximate solutions, of mean-field type, have early been advanced,[5] which helped to gain insight into the mechanism of the phase transition. A new mean-field approach is presented in this paper, in an attempt to clarify the nature of the phase transition in the Ising model. This approach might be considered perhaps as being inspired by the classical work of Peierls.[6]

The energy of an Ising ferromagnet is given by

$$E = -\frac{1}{2} J \sum_{\langle ij \rangle} \mu_i \mu_j \quad , \tag{1}$$

where J is a coupling strength (exchange integral), $\mu_i = \pm 1, i = 1, 2, ... N$, are the spin variables, and N is the number of spins arranged in a d-dimensional lattice, $d = 1, 2, 3$; the summation is extended over the nearest neighbours, such as each spin bond is given the energy $-J$ for parallel spins, and $+J$ for antiparallel spins.

Several approximations will be made herein on the Ising ferromagnet; first, the lattice is replaced by a continuous, uniform distribution of spins, such as each of them interacts with its nearest-neighbours, placed along d orthogonal, local directions. We shall specialize for a while to a two-dimensional lattice, whose ground-state energy is

$$E = -2JN \quad , \tag{2}$$

corresponding to all the N spins aligned. We draw randomly n spins out of N, and reverse them; there are

$$C_N^n = \frac{N!}{n! \, (N-n)!} \tag{3}$$

choices, and we are interested in large N, as for a thermodynamic limit; in addition, we are interested in large values of n, too, such as n/N be constant; for large n the continuum approximation to the spin lattice is a satisfactory approximation.

We proceed now to estimate the change brought in the ground-state energy by reversing n spins. The reversed spins can be arranged in various geometric configurations. For instance, they may be isolated (separated, or "punctual") spins, in which case they change the energy by

$$\delta E_1 = 8Jn \; ; \tag{4}$$

they may be arranged along lines, not necessarily connected, of various shapes and orientations; the energy change brought by such a line of reversed spins is given by

$$\delta E_2 \simeq 4Jn \quad , \tag{5}$$

where the "ends" contribution $(4J)$ can be neglected for large n. One can see easily that a similar energy change proportional to n is brought by several disconnected spin-lines, too. The lines may also intersect with one another, the corresponding energy change being also given by (5). Finally, the reversed spins can be arranged such as to form "islands"; these "islands" may have again various shapes and orientations, and they can also be disconnected, or may intersect with one another. The energy change coresponding to such spins "islands" is $2Jl$, where l is the length of the "islands" boundary, providing the boundary is smooth enough (if not, we get contributions of the type given by (4) and (5), *i.e.* proportional to n). A limiting case of such an "island" corresponds to a "cigar"-like shape; the energy change associated with such a "degenerate island" is proportional to n. Another limiting case of spins "islands" is a quasi-circular "island", whose energy change is given by

$$\delta E_3 = 2Jl \simeq 4J\sqrt{\pi n} \quad . \tag{6}$$

For another type of spins "islands", whose shape differ much of a circle, the corresponding energy will be placed somewhere between $\delta E_3 \sim \sqrt{n}$ and $\delta E_{1,2} \sim n$. We note that the energies of the system can, therefore, be classified according to the types of these independent, geometrical objects consisting of reversed spins; for a given n their energies are continuously distributed between the lowest value $\delta E_3 \sim \sqrt{n}$ and the highest value $\delta E_{1,2} \sim n$; we note also that the largest part of them, that is the largest fraction of their number C_N^n, are such that their behaviour resembles more the dependendece $\sim \sqrt{n}$ than $\sim n$, in the sense that the energy of these states depends on n weaker than n; in fact, the states whose energies go like n are only "marginal" states, the great majority of the states having energies that are weaker than n; the number of perfectly circular "islands", whose energies are exactly of the type $\sim \sqrt{n}$, is also very small in comparison with the rest of states. This peculiarity of the system, namely that of having the energies of almost all of its states behaving weaker than n, has important consequences on the thermodynamical behaviour of the system. The energies of all these states are in fact parametrized by the length l of the geometrical objects (the border length for spins "islands", the length of the spins lines, the "length" of the separated spins being defined as the number of spins); had we were able to know the multiplicity of the geometrical objects with a given l, then we were able to compute the partition function. However, we can obtain an insight into the qualitative behaviour of the system by using the remarks made above.

Indeed, at lower temperatures the "weaker" states might not be activated at all, as their energy is too low; in fact, the energies of these "weaker" states have not a thermodynamic character, in the sense that they go weaker than $\sim n = Nx$, where $x = n/N$ is the fraction of the reversed

spins; for instance, $\sqrt{n} = \sqrt{N} \cdot \sqrt{x}$, which correspond to a vanishing energy per spin in the thermodynamic limit $N \to \infty$. At low temperatures the "weaker" states may not be able to ensure a thermodynamic behaviour of the system. Only for higher temperatures, when higher-energy states come into play, *i.e.* those states whose energies are closer to $\sim n$, the system may acquire a "good" thermodynamics. This may indicate a phase transition, as, in fact, we expect in these systems.

The mean-field assumption to be made presently is suggested by the following remark. Since the energy of the geometrical objects depends only on their length l, we may write the ground-state energy (2) as $E = -2JN = -2\pi JR^2 = -JRL$, where R is the radius and $L = 2\pi R$ is the length of the circle with area $N = \pi R^2$, and compute its small variations as

$$\delta E = 2JR\delta L = 4\pi JR\sqrt{n/\pi} = 4\pi J\sqrt{N/\pi}\sqrt{n/\pi} = 4J\sqrt{Nn} \tag{7}$$

for quasi-circular "islands" (the extra factor -2 in δE comes from the spin reversal); comparing this energy change with δE_3 given by (6) for one "island" we can see that (7) amounts to taking together $\delta E/\delta E_3 = \sqrt{N/\pi}$ "islands", and assume that they behave as one statistical entity whose energy has a correct thermodynamic character: indeed, $\sqrt{Nn} \sim Nx$. This suggests to divide all the "weaker" states in groups, such as the total energy of each group be approximately $\delta E = 4J\sqrt{Nn}$, and assume that each group behaves as an autonomous statistical entity. Each group includes lesser and lesser states, as we go from the quasi-circular "islands" to the "marginal" states corresponding to spin lines or to separated spins, while their energy is not much distorted by replacing it with $\delta E = 4J\sqrt{Nn}$; indeed, the spin lines, whose group multiplicity is unity, has an energy $\delta E_2 \simeq 4Jn$, which does not differ too much from $\delta E = 4J\sqrt{Nn}$, providing $x = n/N$ is not very small; the same conclusions holds also for separated spins, where $\delta E = 4J\sqrt{Nn}$ is to be compared with $\delta E_1 = 8Jn$. We assume, therefore, that every group of states brings an energy change $\delta E = 4J\sqrt{Nn}$. The assumption that all the "weaker" states in each group behave like one statistical object is the main assumption of the mean-field theory; it implies that all the states belonging to a group are correlated in a certain sense. We emphasize that such a mean-field assumption is only meant to describe qualitatively, and in thermodynamical terms, a possible phase transition in the system, but we should be aware that it may lead to unrealistic quantitative results, in virtue of its rather arbitrary character. The arbitrariness comes from the assumption that the "weaker" states in each group are correlated and behave as one statistical entity. The multiplicity of various groups is obtained by dividing the corresponding number of states by the factor by which we have multiplied the energy of those states; for instance, the multiplicity of the groups containing the quasi-circular "islands" is the number of the quasi-circular "islands" divided by $\delta E/\delta E_3 = \sqrt{N/\pi}$, while the multiplicity of the "marginal" states is unity. These dividing factors decrease, therefore, gradually on passing from the "weakest" states (quasi-circular "islands") to less "weaker" states. The total number of states is given by C_N^n in (3), and on comparing this number with the dividing factors, we can see that the latter do not change significantly the total number of states; in other words, the total number of groups can be taken as being the same as the total number of states; this is indeed reasonable, since the largest groups are made of the scarcest states (quasi-circular "islands"). We may assume therefore that the groups multiplicity is C_N^n.

With these assumptions we can pass now to compute the partition function of the system,

$$Z = \frac{1}{2^N} \int dn \cdot e^{-4J\beta\sqrt{Nn} + \ln C_N^n} \quad , \tag{8}$$

where $\beta = 1/T, T$ being the temperature. Using the Stirling formula we can recast the partition function as

$$Z = N \int_0^1 dx \cdot f(x) \quad , \tag{9}$$

where

$$f(x) = e^{\Phi(x)} \quad , \quad \Phi(x) = -4J\beta N\sqrt{x} - Nx \ln x - N(1-x) \ln(1-x) - N \ln 2 \quad . \tag{10}$$

We estimate the integral in (9) by the method of the steepest descents. Equation

$$\Phi'(x) = -\frac{2J\beta N}{\sqrt{x}} + N \ln\left(\frac{1}{x} - 1\right) = 0 \tag{11}$$

has no solution for $J\beta$ larger than a certain critical value $J\beta_c$, and has two solutions (one evolving rapidly to zero, and another, denoted by x_0, evolving rapidly to 1/2) for $J\beta$ smaller than $J\beta_c$. The critical temperature $T_c = 1/\beta_c$ is given by

$$\Phi'(x_c) = -\frac{2J\beta_c N}{\sqrt{x_c}} + N \ln\left(\frac{1}{x_c} - 1\right) = 0 \quad ,$$

$$\Phi''(x_c) = \frac{J\beta_c N}{x_c \sqrt{x_c}} - \frac{N}{x_c(1-x_c)} = 0 \quad . \tag{12}$$

We obtain from these equations the critical concentration of reversed spins $x_c = 0.1$ and the critical temperature given by $J\beta_c = 0.35$. It is noteworthy how close is this critical temperature to the exact value $J\beta_c = 0.44$.[3]

At high temperatures $(J\beta \ll J\beta_c)$ the function $f(x)$ is highly peaked on x_0 close to 1/2 in the thermodynamic limit $N \to \infty$, and the system has a "good" thermodynamics: the steepest descents work, the distribution $f(x)$ has a dispersion $\sim 1/\sqrt{N}$. In this limit $x_0 \cong \frac{1}{2}\left(1 - \sqrt{2}J\beta\right)$ and the magnetization

$$M = mN(1 - 2x) \sim 1/T \quad , \tag{13}$$

i.e. we obtain the Curie law; m in (13) denotes the magnetic moment of one spin. The free energy in this case is given by

$$-\beta F = -4J\beta N\sqrt{x_0} - Nx_0 \ln x_0 - N(1-x_0) \ln(1-x_0) - N \ln 2 \quad , \tag{14}$$

and we obtain the specific heat $c \sim 1/T^2$.

On decreasing the temperature, and approaching the critical temperature, the distribution $f(x)$ flattens gradually, and the "good" thermodynamics is degraded. The fluctuations diverge, and below the critical point the function $f(x)$ vanishes, while being peaked at $x = 0$; similarly, the partition function vanishes, in the thermodynamic limit.[7] Consequently, the only acceptable solution for $\beta > \beta_c$ is $x = 0$, *i.e.* the system is ferromagnetically ordered with $M = mN$. At the critical temperature the mgnetization has a sudden fall at $mN(1-2x_c)$, followed by a rapid decrease to zero. We obtain easily from (11) and (12) $x_0 - x_c \cong (\beta_c - \beta)^{1/2}$; hence, the magnetization has an infinite slope at T_c, of the form $\sim -(T - T_c)^{-1/2}$. Though irrelevant, we compute nevertheless, as usually, the free energy slightly above the critical temperature, and obtain the specific heat $c \sim (T - T_c)^{-1/2}$, *i.e.* the specific heat has an infinite jump at the critical tempearture (c vanishes for $T < T_c$). The free energy and the energy are continuous at T_c. All these results are typical for a mean-field theory.

Similar results are obtained for the three-dimensional system. The energy associated with the two-dimensional "islands" has now a thermodynamic character, *i.e.* it goes like n. It is the three-dimensional "islands" now that are very peculiar, in the sense that their energy is "'weaker" than n; the energy of quasi-spherical "islands" is, for instance, $\delta E_4 = 2 \left(36\pi\right)^{1/3} Jn^{2/3}$. Taking into account the variation of the surface associated with such three-dimensional "islands" we get the energy

$$\delta E = 6JN^{1/3}n^{2/3} \quad , \tag{15}$$

such that the partition function is given by

$$Z = \frac{1}{2^N} \int dn \cdot e^{-6J\beta N^{1/3}n^{2/3} + \ln C_N^n} \quad . \tag{16}$$

Following the same procedure as above we obtain the critical concentration $x_c = 0.04$, and the critical temperature given by $J\beta_c = 0.27$; we note again that this value is very close to 0.22, considered as being practically the exact value for the simple cubic lattice.[4] The magnetization and the specific heat have the same "critical exponents" as in the two-dimensional case.

We note finally that non-thermodynamic states, *i.e.* states whose energy is "weaker" than n, do not exist in one-dimension, where there is no transition.

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