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Phase diagrams of random Ising models: 
simple and systematic successive approximations

A. Benyoussef (*) and N. Boccara

SPSRM, CEN-Saclay, 91191 Gif sur Yvette, France

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Abstract. — We present a simple and systematic method to calculate phase diagrams of random Ising models. It applies to a wide class of systems in which, however, randomness has to be described by discrete random variables. We calculated, at different orders of approximation, various quantities like critical temperatures and percolation thresholds in good agreement with exact known results.


Consider the Ising Hamiltonian

$$H = J \sum_{\langle i,j \rangle} \sigma_i \sigma_j$$

where $J > 0$, $\sigma_i = \pm 1$ and the summation runs over all pairs of nearest neighbours.

If $\langle \sigma_0 \rangle_c$ denotes the mean value of $\sigma_0$ for a given configuration c of all other spins, i.e. when all other spins $\sigma_i$ ($i \neq 0$) have fixed values, we have

$$\langle \sigma_0 \rangle_c = \frac{\text{tr} \sigma_0 \exp - \beta H}{\text{tr} \exp - \beta H} \left( \beta = \frac{1}{T} \right)$$

$$= \tanh \left( K \sum_{i=1}^{z} \sigma_i \right),$$

where $K = \beta J$ and the summation is extended over the $z$ nearest neighbours $\sigma_i$ ($i = 1, 2, ..., z$) of $\sigma_0$. This relation is exact and the magnetization per site, which is the thermal average $m$ of $\sigma_0$, is obtained by averaging $\tanh \left( K \sum_{i=1}^{z} \sigma_i \right)$ over all configurations.

This is a formidable task and the mean-field approximation corresponds to the very crude estimate

$$\tanh \left( K \sum_{i=1}^{z} \sigma_i \right) \approx \tanh K z m ,$$

which gives a critical temperature $T_c = zJ$. In the case, for example, of a honeycomb lattice ($z = 3$) this result compares rather poorly with the exact one [4]

$$T_c = \frac{2J}{\ln (2 + \sqrt{3})} = 1.519 J .$$

To obtain a better result we make use of the following property: a function defined on a finite set is equal to a polynomial. In the considered case we have \(^{(1)}\)

\(^{(1)}\) Cf. theorem given at the end of this section.
\[ \tanh K(\sigma_1 + \sigma_2 + \sigma_3) = \frac{1}{2}(\tanh 3K + \tanh K)(\sigma_1 + \sigma_2 + \sigma_3) + \frac{1}{4}(\tanh 3K - 3 \tanh K)\sigma_1 \sigma_2 \sigma_3. \tag{2} \]

If now we average the right-hand side of (2) approximating \( \langle \sigma_1 \sigma_2 \sigma_3 \rangle \) by \( m^3 \), we obtain the equation

\[ m = \frac{3}{4}(\tanh 3K + \tanh K)m + \frac{1}{4}(\tanh 3K - 3 \tanh K)m^3, \tag{3} \]

which determines \( m \) in the whole temperature range.

Within this approximation the critical temperature is the solution of

\[ 1 = \frac{3}{4}(\tanh 3K + \tanh K), \tag{4} \]

i.e. \( T_c = 2.10 J \), which is better than the mean field result.

The reason why this method gives a better result than the ordinary mean-field approximation is due to the fact that it takes exactly into account relations like \( \sigma_i^2 = 1 \) and, as a consequence, neglects only correlations between different random variables. On the contrary, averaging a relation like (1), the mean-field approximation neglects all correlations.

In other words, the ignored probability law \( P(\{ \sigma_i \}) \) of the set of random variables \( \{ \sigma_i \} \) is, in this method, taken equal to

\[ \prod_i \left( \frac{1 + m}{2} \delta(\sigma_i - 1) + \frac{1 - m}{2} \delta(\sigma_i + 1) \right) \]

while the mean-field approximation corresponds to

\[ P(\{ \sigma_i \}) = \prod_i \delta(\sigma_i - m). \]

At this point it is interesting to note that the method is exact for a one-dimensional Ising model for, in this case,

\[ \langle \sigma_0 \rangle_c = \tanh K(\sigma_1 + \sigma_2) \]

\[ = \frac{1}{2}(\sigma_1 + \sigma_2) \tanh 2K \]

which, after averaging, gives

\[ m = m \tanh 2K \]

i.e.

\[ m = 0 \] \( \text{if} \ T \neq 0 \) \( \text{tanh} \ 2K \neq 1 \).

It is not difficult to derive the equation which determines the critical temperature for any number \( z \) of nearest neighbours if one uses the following theorem:

the set of all bounded real functions of \( \sigma_1, \sigma_2, ..., \sigma_z \) is a \( 2^z \)-dimensional Euclidean space. The set \( \{ 1, \sigma_1, ..., \sigma_1 \sigma_2, ..., \sigma_1 \sigma_2 \sigma_z \} \) which contains all the products of different spins is an orthonormal basis for the inner product defined by

\[ \langle f_1 | f_2 \rangle = \]

\[ = \frac{1}{2^z} \text{tr} f_1(\sigma_1, \sigma_2, ..., \sigma_z) f_2(\sigma_1, \sigma_2, ..., \sigma_z), \]

\[ \tanh \left( K \sum_{i=1}^z \sigma_i \right) \] being invariant by permutations of the \( \sigma_i \)'s, the equation for the critical temperature reads

\[ 1 = \frac{z}{2^z} \text{tr} \sigma_1 \tanh \left( K \sum_{i=1}^z \sigma_i \right) \]

\[ = \frac{z}{2^z-1} \sum_{l=0}^{z-1} \frac{(z-1)}{l} \tanh (z-2l)K. \]

In what follows we shall consider only the case \( z = 3 \) in order to simplify the calculations. At the same time this case is a good test for the method. Increasing \( z \) leads, for the critical temperature, to a better agreement between approximate and exact results.

The same method could be used to study many other pure Ising models with, for example, applied external fields, different interactions or spins greater than \( \frac{1}{2} \).

2. Pure Ising models. nth order approximation.

The zeroth order approximation for the expression of \( \langle \sigma_0 \rangle_c \) has been obtained performing the traces over \( \sigma_0 \), all other spins of the lattice having fixed values. We shall define the first-order approximation for \( \langle \sigma_0 \rangle_c \) performing the traces over \( \sigma_0 \) and its first neighbours \( \sigma_1, \sigma_2 \) and \( \sigma_3 \), all other spins of the lattice having fixed values. It is clear that the expression of \( \langle \sigma_0 \rangle_c \) in this case will depend only on the spins \( \sigma_4, \sigma_5, \sigma_6, \sigma_7, \sigma_8 \) and \( \sigma_9 \) (Fig. 1) which are the external first neighbours of the spins belonging to the border of the cluster \( \{ \sigma_0, \sigma_1, \sigma_2, \sigma_3 \} \). Taking into account the theorem given in the preceding section, \( \langle \sigma_0 \rangle_c \) can be written in the form of a polynomial and then averaged as we did for the zeroth order approximation.

We shall not write down explicitly the equation \( m = f(K, m) \) which is rather complicated.

The second order approximation for \( \langle \sigma_0 \rangle_c \) is defined with traces performed over the spins belonging to the cluster \( \{ \sigma_0, \sigma_1, ..., \sigma_9 \} \) and more generally the \( n \)th order approximation is defined, in an obvious way, by traces performed on all the spins of a cluster centred on \( \sigma_0 \) which contains

\[ 1 + 3 + 6 + \cdots + 3n = 1 + \frac{3n(n + 1)}{2} \text{spins}, \]

all the spins of the lattice not belonging to the cluster having fixed values. The expression of \( \langle \sigma_0 \rangle_c \), which
Fig. 1. — (a) Cluster used for the first order approximation. 
(b) Cluster used for the second order approximation.

is exact, depends only on the external first neighbours of the spins of the border of the considered cluster. Here again, after having written \( \langle \sigma_0 \rangle_c \) in polynomial form, we average this last expression neglecting correlations between different spins.

In order to test the convergence of these successive approximations, we calculated the critical temperature for \( n = 1, 2, 3 \) and 4. The results are given in table I.

Using a computer and extrapolation techniques like Pade's we could obtain very precise results. Such techniques could also give the values of critical exponents. This has not been our purpose here.

Table I. — Successive approximations for the critical temperature of the honeycomb Ising model.

<table>
<thead>
<tr>
<th>( n )</th>
<th>0</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>exact</th>
</tr>
</thead>
<tbody>
<tr>
<td>( T_c(n) )</td>
<td>2.10</td>
<td>1.91</td>
<td>1.84</td>
<td>1.78</td>
<td>1.73</td>
<td>1.52</td>
</tr>
</tbody>
</table>


Extension of this method to the less trivial case of random models is straightforward. If, for instance the reduced interactions \( K_{ij} \) are random variables, the mean value of \( \sigma_0 \) when all other spins \( \sigma_i (i \neq 0) \) and all interactions \( K_{ij} \) have fixed values is, for \( z = 3 \), given exactly by

\[
\langle \sigma_0 \rangle_c = \tanh (K_{01} \sigma_1 + K_{02} \sigma_2 + K_{03} \sigma_3) \\
= A_1 \sigma_1 + A_2 \sigma_2 + A_3 \sigma_3 + B \sigma_1 \sigma_2 \sigma_3,
\]

where

\[
A_1 = \frac{1}{4} \tanh (K_{01} + K_{02} + K_{03}) + \tanh (K_{01} - K_{02} - K_{03}) + \tanh (K_{01} - K_{02} + K_{03}) + \tanh (K_{01} + K_{02} - K_{03})
\]

and

\[
B = \frac{1}{4} \left[ \tanh (K_{01} + K_{02} + K_{03}) + \tanh (K_{01} - K_{02} - K_{03}) + \tanh (K_{01} - K_{02} + K_{03}) + \tanh (K_{03} - K_{01} - K_{02}) \right].
\]

For a bond dilute model \( K_{0i} = Kn_i \) where \( n_i \) is the occupation number of bond 0i. The coefficients \( A_i (i = 1, 2, 3) \) and \( B \) in (5), as functions of \( n_1, n_2 \) and \( n_3 \), are equal to polynomials, and here again neglecting correlations between different random variables, we can approximately average the right hand side of (5). This yields

\[
m = 3 A(p, K) m + B(p, K) m^3,
\]

with

\[
A(p, K) = \frac{1}{4} \left[ (4p - 8p^2 + 5p^3) \tanh K + 4(p^2 - p^3) \tanh 2K + p^3 \tanh 3K \right] \quad (7)
\]

\[
B(p, K) = \frac{1}{4} p^3 (\tanh 3K - 3 \tanh K), \quad (8)
\]

where \( p = \langle n_i \rangle \) is the bond concentration. The second order transition line (Fig. 2a) is determined by

\[
1 = 3 A(p, K),
\]

Fig. 2. — Phase diagram for a bond dilute honeycomb Ising model. (a) 0th order approximation; (b) 1st order approximation.
and the bond percolation threshold $p_B^*$ by
\[
1 = \lim_{K \to \infty} 3 A(p, K) = \frac{1}{4} (4p - 4p^2 + 2p^3),
\]
i.e. $p_B^* = 0.557$ which is rather good compared to the exact result $p_B^* = 0.6527$ [5].

The site problem, which is usually more difficult, can be treated as easily as the bond problem. Here $K_{oi} = Kn_i n_i$ where $n_0$ and $n_i$ are the occupation numbers of sites 0 and $i$. A simple calculation yields the equation
\[
m = 3 A(p, K) m + pB(p, K) m^3
\]
where $A(p, K)$ and $B(p, K)$ are still given by (7) and (8) but where $p$ is now the site concentration. The equation of the second order transition line (Fig. 3a) is
\[
1 = \tfrac{3}{2} (4p^2 - 4p^3 + 2p^4)
\]
is equal to 0.801 to be compared to $p_B^* = 0.698 \pm 0.003$ obtained by series expansion [6].

Frustrated systems in which the nearest-neighbour interactions are either ferro- or antiferromagnetic are also easy to treat. In this case $K_{oi} = K_{ei}$ with $e_i = \pm 1$ and a simple calculation shows that the magnetization per site is determined by the equation
\[
m = \frac{1}{4}(1 - 2c) (\tanh 3K + \tanh K) m + \frac{1}{4}(1 - 2c)^3 (\tanh 3K - 3\tanh K) m^3
\]
where $c = \frac{1}{2}(1 - \langle e \rangle)$ is the concentration of negative interactions. The corresponding phase diagram for the para-ferromagnetic phase transition is represented on figure 4a. This phase diagram exhibits a concentration threshold $c^* = \frac{1}{2}$ of antiferromagnetic bonds above which ferromagnetic order cannot exist. The exact value of $c^*$ is not known.

The phase diagram for the para-antiferromagnetic transition is obtained changing $c$ in $1 - c$.

We could combine frustration and dilution to obtain $(T, p, c)$ phase diagrams. If, for example, we consider bond dilution, we have $K_{oi} = Kn_i e_i n_i$ and $e_i$ having the same meaning as before, and a straightforward calculation yields the equation
\[
m = 3 A(p, c, K) m + B(p, c, K) m^3
\]
with
\[
A(p, c, K) = p(1 - 2c) \tanh K + p^2(1 - 2c) (\tanh 2K - 2\tanh K) + \frac{1}{4} p^3(1 - 2c) (\tanh 3K - 4\tanh 2K + 5\tanh K)
\]
\[
B(p, c, K) = \frac{1}{4} p^3(1 - 2c)^3 (\tanh 3K - 3\tanh K).
\]
We have calculated first order corrections for all the cases we have considered. The resulting phase diagrams are represented in figures 2b, 3b and 4b.

The thresholds for this first order approximation are

\[ p_B^* = 0.581 \quad p_S^* = 0.744 \quad \text{and} \quad \epsilon^* = 0.135. \]

As expected the values for \( p_B^* \) and \( p_S^* \) are in better agreement with the exact ones.

4. Conclusion.

We have presented a simple and systematic method to calculate phase diagrams of random Ising models, We applied it to diluted and frustrated systems. Numerical agreement with exact known results are very satisfactory. The method applies only to systems in which randomness can be described by discrete random variables. Its application needs also the knowledge of the order parameter characterizing the phase transition.

We have not studied spin-glass phase transitions. We could have done it; but in that case, in order to introduce an order parameter, we should have to consider either the Mattis model [7] which is not believed to describe a spin-glass system correctly or the Edwards-Anderson one [8] and in this case we would have been led to use the questionable replica trick making the method loose its simple character.

References


