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# Cluster Perturbation Theory for 2d Ising Model

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*This paper deals with 2d Ising model in the scope of cluster perturbation theory. Ising model is defined on a two-dimensional square lattice, the amount of nearest neighbors z=4. Lattice is divided into clusters of a given size and a complete set of energy eigenvalues and eigenvectors of the cluster is defined by the diagonalization method. On the basis of this, Hubbard operators are constructed and Green function is calculated, taking into account intercluster interactions according to perturbation theory, it allows us to obtain the dependence of the magnetization on the temperature in the Hubbard-I approximation. Obtained results are compared with the exact solution of the two-dimensional Ising model.*

*Keywords: cluster perturbation theory, Ising model, X-operators.*

## Introduction

As is known, Ising model is one of the basic model of the statistical physics and is used for ferromagnets description. The presence of and exact solution in one- and two- dimensional cases is one of the main advantages of this model, it allows us to check numerical methods of solving statistical physics problems using it.

In the two-dimensional case Ising model was exactly solved by Onsager in 1944 [1]. Expression for spontaneous magnetization was obtained by Onsager in 1949 and the full derivation was represented by Yang in 1952 [2]. In the isotropic case the spontaneous magnetization has the following form

$$M = \left(1 - \sinh^{-4}\left(\frac{J}{kT}\right)\right)^{1/8},$$

where $k$ is for Boltzmann constant. The value of the critical exponent $\beta = 1/8$, and the critical temperature $T_c = \dfrac{J}{k}\dfrac{1}{\ln(1+\sqrt{2})} \approx 1.135\dfrac{J}{k}$.

In the case of mean-field theory (In this case it is corresponding to Hubbard-I decoupling) results correspond to exact solution badly. The amount of critical exponent $\beta$ and critical temperature are, respectively $\beta = 1/2$ and $T_c = 2$.

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Over last two decades much attention is paid to the cluster approach during lattice models study [3]. In this paper Cluster Perturbation Theory (CPT), previously used in the solution of Hubbard model [4]. In this approach the representation of $X$-operators is used [5], on the basis of which the Hubbard Green's function is constructed and the average amount of spin is calculated.

# 1. Method

The Hamiltonian of the Ising model

$$H = -\frac{1}{2}\sum_{i,j} J_{ij} S_i^z S_j^z - h\sum_i S_i^z,$$

where $J_{ij} = J$ for the nearest neighbours and is zero for non-nearest neighbours, $h$ is the external field, $S_i^z$ is spin projection. By dividing the lattice into clusters (Fig. 1) and rearranging the terms so as to separate intra-cluster and inter-cluster interaction, we get:

$$H = \sum_i H_0(i) + \sum_{ij} H_1(i,j),$$

where $H_0(i)$ is the intra-cluster part of the $i$-th cluster. This term is exactly diagonalized and on the basis of its eigenvectors Hubbard operators are constructed. $H_1(i,j)$ are interactions between cluster $i$ and $j$.

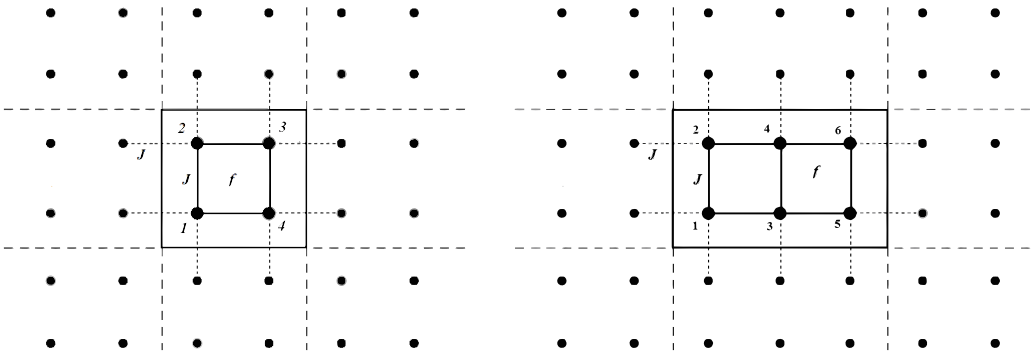


Fig. 1. Cluster 2x2 (left) and cluster 3x2 (right)

The Hubbard operators used in the paper (X-operators) are described in more detail in [5]. Operators $S^+$, $S^-$ and $S^z$ can be represented by X-single-site operators, such as

$$S^+ = X_f^{+-},$$
$$S^- = X_f^{-+},$$
$$S^z = \frac{1}{2}\left(X_f^{++} - X_f^{--}\right).$$

In general operator $X^{pq}$ is a matrix whose elements are equal to zero, except for one, standing on the intersection of the $p$ and $q$-line and equal to 1

$$X^{pq} = |p><q|.$$

The action of such operator defines the system transition from $q$ state to state $p$. Thus there are $2^N$ state ($N$ is for amount of nodes in the cluster), each of them corresponds to one state of cluster ($2 \times 2$ cluster for example ):

$$|1>=|\uparrow,\uparrow,\uparrow,\uparrow>$$
$$|2>=\frac{1}{2}\left(|\downarrow,\uparrow,\uparrow,\uparrow>+|\uparrow,\downarrow,\uparrow,\uparrow>+|\uparrow,\uparrow,\downarrow,\uparrow>+|\uparrow,\uparrow,\uparrow,\downarrow>\right)$$
$$\ldots$$
$$|16>=|\downarrow,\downarrow,\downarrow,\downarrow>.$$

In this representation spin operators in the cluster $f$ on the atom $n = 1, ..., N$ have the following form:

$$S^z_{fn} = \sum_p \gamma_{pn} X^{pp}_f,$$

where the matrix element $\gamma_{pn}$ are calculated directly, knowing the exact states of the cluster.

$$\gamma_{pn} =< p|S^z_n|p > .$$

From the point of view of Hubbard operators the new Hamiltonian has the following form:

$$H = \sum_{f,p} \epsilon_p X^{pp}_f + \sum_{fg} \sum_{pq} \sum_{nm} \gamma_{pn}\gamma_{qm} J^{pq}_{fg} X^{pp}_f X^{qq}_g, \tag{1}$$

where $\epsilon_p$ are eigenvalues energy of the cluster, $J^{pq}_{fg}$ are interaction energy between clusters $f$ and $g$ in the states $p$ and $q$ respectively.

Two-time Green functions are constructed to get the magnetization:

$$G(t,t') =\ll A(t)|B(t') \gg= \theta(t-t') < [A(t), B(t')] >,$$

where $\theta(t-t')$ is theta-function (Heviside function). The equation for the function is written as:

$$E \ll X^{mn}_f|X^{rs}_g \gg =< [X^{mn}_f, X^{rs}_g] > + \ll [X^{mn}_f, H]|X^{rs}_g \gg . \tag{2}$$

Green function, which stands in the right part is more complex and has the form $\ll X^{mn}_f X^{pq}_h|X^{rs}_g \gg$. It is necessary to record the same equation for this functions for exact solution, which in turn leads to a chain of coupled equations. In this paper approximation Hubbard-I, which is to facilitate the Green function, is used to disengaged the chain:

$$\ll X^{mn}_f X^{pp}_h|X^{rs}_g \gg =< X^{pp}_h > \ll X^{mn}_f|X^{rs}_g \gg, \tag{3}$$

which allows to close the chain of equations. It should be noted that Hubbard-I approximation corresponds to the mean-field approximation for the Ising model. In non-cluster case, the obtained solution correspond to well-known solution of the theory of Landau.

Explicitly the Green function obtained from the equation (2), with (1) and (3), has the following form:

$$\ll X^{pq}_f|X^{qp}_g \gg = \frac{< X^{pp} > - < X^{qq} >}{E + \epsilon_p - \epsilon_q - 2J\sum_{j,m}\sum_{rs}\gamma_{mr} < X^{mm} > \left(\gamma_{qs}J^{mq}_{fj} - \gamma_{ps}J^{mp}_{fj}\right)}.$$

Using the spectral theorem, we will find the occupation numbers $< X^{pp}_f >$:

$$< X_f^{pq} X_f^{qp} >=< X_f^{pp} >= \lim_{\delta \to 0} \frac{1}{2^N} \sum_q \int \frac{1}{e^{\beta E} - 1} \left( \frac{i}{\pi} \right) Im \left( \ll X_f^{pq} | X_g^{qp} \gg_{E+i\delta} \right) dE,$$

where $\beta = \dfrac{1}{kT}$. This we obtain the system of $2^N$ equations, by solving which we will obtain the occupation numbers.

Because we obtain 16 equations even for $2 \times 2$ clusters, their solution is carried out numerically, after taking normalization conditions into account:

$$\sum_p X_f^{pp} = 1,$$

average amount of spin(magnetization) is calculated:

$$< S^z >= \frac{1}{N} \sum_{p,j} \gamma_{pj} < X_f^{pp} > .$$

## 2. Critical temperature and critical exponent $\beta$

We have considered numerical solution of the model for a number of square clusters $n \times n$ for $n^2 = N$ up to $N = 16$. Normal mean-field approximation is obtain for N=1. The values of magnetization obtained as a result of calculation are presented in Fig. 2.

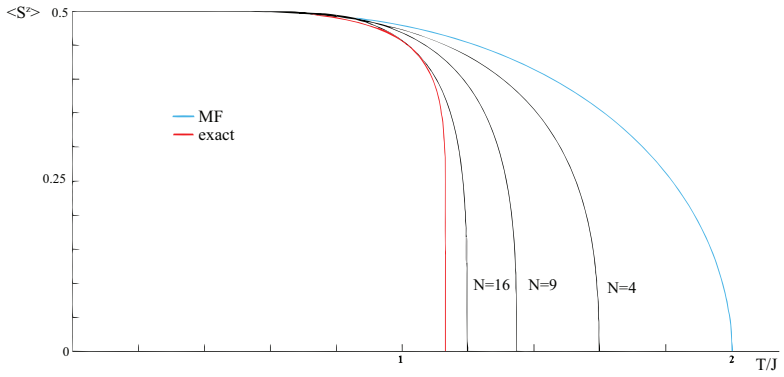


Fig. 2. The average amount of spin projection $S^z$ in dependence on the temperature and cluster size. Blue color indicates the solution in the mean-field approximation, red color is the exact solution, black color is the solution for different values of the cluster size

The obtained values of critical temperature are shown in Tab. 1.

Table 1.

| N | 1 (MF) | 4 | 6 | 9 | 12 | 16 | 20 | 25* | 30* | exact |
|---|---|---|---|---|---|---|---|---|---|---|
| $kT_c/J$ | 2 | 1.596 | 1.451 | 1.347 | 1.259 | 1.197 | 1.162 | 1.15 | 1.145 | 1.135 |

* is approximated value.

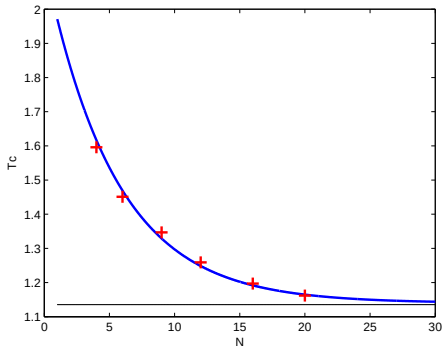


Fig. 3. The dependence of the critical temperature on the cluster size. The blue line corresponds to the approximated curved line, the "+"corresponds to the calculated values, the black direct line corresponds to the precise value.

The dependence of the critical temperature on the cluster size can be approximated by the following function:

$$\frac{k(T_c(N) - T_c(exact))}{J} = e^{-0.185N}.$$

The obtained values of critical exponent $\beta$ do not depend on the size of cluster and are equal to 1/2, at the same time index $\beta = 1/8$ gives the exact solution. Function $\beta(T)$ is introduced for the behaviour of magnetization curve analysis

$$\beta(T) = \frac{d(\ln < S^z >)}{d(\ln(k(T_c - T)/J))}.$$

Also in should be noted that:

$$\lim_{T \to T_c} \frac{d(\ln < S^z >)}{d(\ln(k(T_c - T)/J))} = \beta.$$

The values of $\beta(T)$ obtained as a result of calculation are presented in Fig. 4.

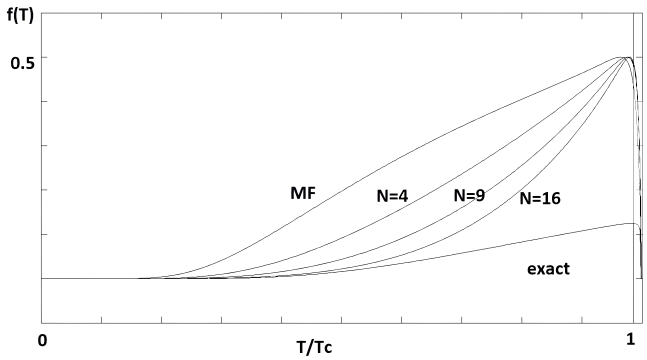


Fig. 4. Diagram of the dependence of the function $\beta(T)$ on the size of cluster $N$

The graphic shows that if $N$ is increasing in the temperature range $T < T_c$ the curve $f(T)$ approaches to exact solution, but at the transition point the exponent $\beta$ would be equal to $1/2$ for any finite size of the cluster. This is due to the fact that the correlations length of $T_c$ tends to infinity, while this method is to the correlations length equivalent to the size of the cluster. Thus, at the phase transition point the size of cluster does not matter, since it is infinitely smaller than the correlations length.

## Conclusion

In conclusion of this paper the advantage of the calculation speed of this method with respect to the Monte-Carlo Method, which is used for calculation of magnetization in the Ising mode, should be noted. The time of calculation in the Monte-Carlo method is proportional to the size of cluster as:

$$t_{MC} \sim N,$$

while the time of calculation the cluster perturbation theory is

$$t_{CPT} \sim 2^N.$$

On the other hand, the mistake in the calculation of the critical temperature:

$$\frac{k\delta T_{MC}}{J} \sim \frac{1}{\sqrt{N}},$$

$$\frac{k\delta T_{CPT}}{J} = e^{-0.185N}.$$

Thus:

$$t_{MC} \sim \frac{1}{(k\delta T_{MC}/J)^2},$$

$$t_{CPT} \sim \frac{1}{(k\delta T_{CPT}/J)^{3.747}}.$$

Calculations show, that for the same accuracy, which corresponds to $4 \times 4$ for CPT and $300 \times 300$ for MC time ratio of calculating by method of cluster perturbation theory and Monte-Carlo method are respectively equal

$$\frac{t_{MC}}{t_{CPT}} \simeq 10.$$

This shows that for small cluster sizes CPT is more effective than Monte-Carlo theory, which provides a speed advantage only for big cluster sizes.

Our comparison of the exact and CPT solutions has revealed that for a lattice of $4 \times 4$ clusters the deviation of thermodynamics from the exact occurs at $T/T_c > 0.5$, while for standard mean field theory it starts (as can be seen from the fig.3) at $T/T_c > 0.2$. Obviously the reason of better behavior of CPT over standard mean-field approach is exact accounting for the short range magnetic order inside the cluster.

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## Кластерная теория возмущений для двумерной модели Изинга

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*В настоящей работе проводится исследование двумерной модели Изинга в рамках кластерной теории возмущений. Модель Изинга задана на двумерной квадратной решетке с числом ближайших соседей z=4. Решетка разбивается на кластеры заданного размера и методом точной диагонализации определяется полный набор собственных значений энергии и собственных векторов кластера. На этом базисе строятся операторы Хаббарда и вычисляется функция Грина с учетом межкластерных взаимодействий по теории возмущений, позволяющая получить зависимость намагниченности от температуры в приближении Хаббард-I. Полученные результаты сравниваются с точным решением двумерной модели Изинга.*

*Ключевые слова: модель Изинга, кластерная теория возмущений, X-операторы.*