УДК 538

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Розрахунок фазових переходів в одновимірній моделі Ізінга методом розкладу за сингулярними значеннями

Новий ефективний метод для розрахунку фазових діаграм одновимірних квантових спінових систем використано для моделі Ізінга з поперечним магнітним полем. Отримані результати порівняно з точним аналітичним розв'язком для даної моделі.

Ключові слова: фазові переходи, спінові системи, перенормування матриці густини.

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Calculation of the phase transitions in one-dimensional Ising model using singular value decomposition method

New efficient method for investigation of the phase diagrams of one-dimensional quantum spin-systems applied to standard Ising model with transverse magnetic field. Obtained results are compared with exact analytical answer for this model.

Key Words: phase transitions, quantum spin systems, density matrix renormalization group.

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Introduction

Spin models investigated in this paper are widely used in the theoretical physics. The aim of this paper is to investigate a new and efficient method for studies of the phase diagrams of yet unstudied spin Hamiltonians. The idea of such investigation was first suggested by Anders at al. [1]. The method is based on the singular value decomposition (SVD) of the space correlation tensor (or displacement matrix). For this case SVD is very closely related to the problem of proper orthogonal decomposition (POD), also known as Karjunen-Loeve transform, introduced by Kosambi [2] and to the principal component analysis introduced by Hotelling [3] (See review [4]). POD is a procedure for extracting a basis for a modal decomposition from an ensemble of signals. This is very efficient and optimal method in the sense that for a given number of modes, the projection on the subspace used for modelling the random field will on average contain the most energy possible [5] and given by so called proper orthogonal modes (POMs). Finding of POMs of given physical problem is correlated to the transformation to eigen basis of the given physical model with respect to specific observable (correspondent analogy from mechanics will be the main axe transformation). As it was shown in [5] POD can be carried out by means of singular value decomposition.

Singular value decomposition

Principal component analysis (PCA) is a mathematical procedure that uses an orthogonal transformation to convert a set of observations of possibly correlated variables into a set of values of uncorrelated variables called principal components. The number of principal components is less than or equal to the number of original variables. This transformation is defined in such a way that the first principal component has as high a variance as possible (that is, accounts for as much of the variability in the data as possible), and each succeeding component in turn has the highest variance possible under the constraint that it be orthogonal to (uncorrelated with) the preceding components. Principal components are guaranteed to be independent only if the data set is jointly normally distributed. PCA is sensitive to the relative scaling of the original variables. Depending on the field of application, it is also named the discrete Karhunen-Loe`ve transform (KLT), the Hotelling transform or proper orthogonal decomposition (POD). PCA was invented in 1901 by Karl Pearson [6]. Now it is mostly used as a tool in exploratory data analysis and for making predictive models. PCA can be done by eigenvalue decomposition of a data covariance matrix or singular value decomposition of a data matrix, usually after mean centering the data for each attribute. The results of a PCA are usually discussed in terms of component scores (the transformed variable values corresponding to a particular case in the data) and loadings (the weight by which each standarized original variable should be multiplied to get the component score) .

PCA is the simplest of the true eigenvector-based multivariate analyses. Often, its operation can be thought of as revealing the internal structure of the data in a way which best explains the variance in the data. If a multivariate dataset is visualised as a set of coordinates in a high-dimensional data space (1 axis per variable), PCA can supply the user with a lower-dimensional picture, a “shadow” of this object when viewed from its (in some sense) most informative viewpoint. This is done by using only the first few principal components so that the dimensionality of the transformed data is reduced.

The purpose of singular value decomposition is to reduce a dataset containing a large number of values to a dataset containing significantly fewer values, but which still contains a large fraction of the variability present in the original data. Applying the SVD to space correlation matrix we obtain the most persistent structure of the correlations for each POM. In this paper we use SVD in order to calculate the phase diagrams for 1D Ising model spin chains (rings) in the transverse magnetic field.

XY model with transverse magnetic field

The XY *model with transverse field* for a system of spin-1/2 on a lattice is given by the Hamiltonian

$$H = \sum_{\{a,b\}\in\mathcal{B}} -\frac{1+\gamma}{2}\sigma_z^{(a)}\sigma_z^{(b)} - \frac{1-\gamma}{2}\sigma_y^{(a)}\sigma_y^{(b)} - \sum_{a\in V}\boldsymbol{B}\sigma_x^{(a)}$$

where $\sigma_{x,y,z}$ are the Pauli matrices, $\mathcal{B}$ is the set of all pairs of spins, on which a term act jointly; $\mathcal{B}$ the transverse field and γ is called the asymmetry. For $\gamma = 0$, we get a special case the *XX model* and for $\gamma = 1$, we get the *Ising model*.

As it was shown in [7] for the finite chain the critical regions are: XX criticality at $\gamma = 0$ for $0 < \boldsymbol{B} < 1$ and XY criticality for $\boldsymbol{B} = 1$, $\gamma \neq 0$ (Ising criticality for $\boldsymbol{B} = \gamma = 1$.

The phase diagram which describes the critical regions are shown on Fig. 1.

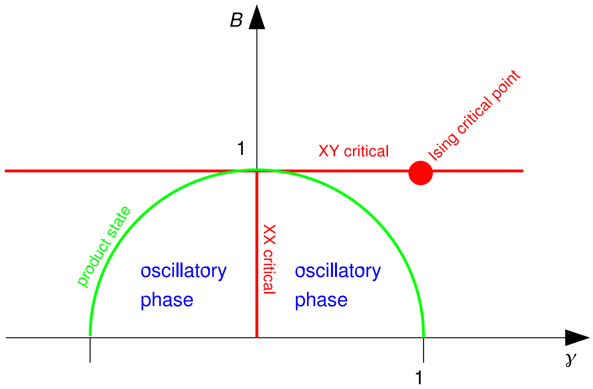

Fig.1 Phase diagram of XY model for 1D spin chain [7] .

Numerical calculations which can confirm the critical behavior of the correlation functions can be done using the DMRG algorithm. Critical behavior of the correlations can be seen from the plots of the singular values of the correlation matrix $\left(\langle\sigma_i^{(a)}\sigma_j^{(b)}\rangle - \langle\sigma_i^{(a)}\rangle\langle\sigma_j^{(b)}\rangle\right)_{i,j=x,y,z}$.

Calculation of the correlation functions separately are not showing yet predicted by [7] phase diagram. Three dimensional plot of correlation functions can be seen from Fig. 3

Rest of the correlation functions $\langle\sigma_x^a\sigma_y^b\rangle$, $\langle\sigma_x^a\sigma_z^b\rangle$, $\langle\sigma_y^a\sigma_z^b\rangle$ and etc. are effectively zero. As we can see our correlations correctly reproduce the analytical predictions made in [7] about vanishing of the correlations while approaching to the points on the Baruch-McCoy circle, which is defined by $\boldsymbol{B}^2 + \gamma^2 = 1$. On this circle the ground state has product form [7]. This behavior can be clearly seen from second and third plots which corresponds to middle and lowest singular values of the correlation matrix respectively. Maximal singular value is not very informative for this type of calculations because of the strong criticality at $\gamma = 0$.

From the Fig. 2 we also can see that critical behavior at $\gamma = 0$ (XX criticality) is much stronger than XY criticality. Ising critical point at $\gamma = \boldsymbol{B} = 1$ do not have that strong critical behavior as at $\gamma = 0$. This picture of the correlation functions behavior is in qualitative agrement with behavior of the amount of entanglement in this regions (See Fig. 3 in [8]).

Calculations of the magnetization M_x and M_z which are given as

$$M_{(z,x)} = \frac{1}{N}\langle 0|\sum_{j-1}^{N}\sigma_{(x,z)}^{j}|0\rangle$$

here |0⟩ in our DMRG calculations is an eigenvector which corresponds to the lowest eigenvalue measured in the middle of the chain. For periodic boundary conditions this condition is irrelevant because of the ring symmetry.

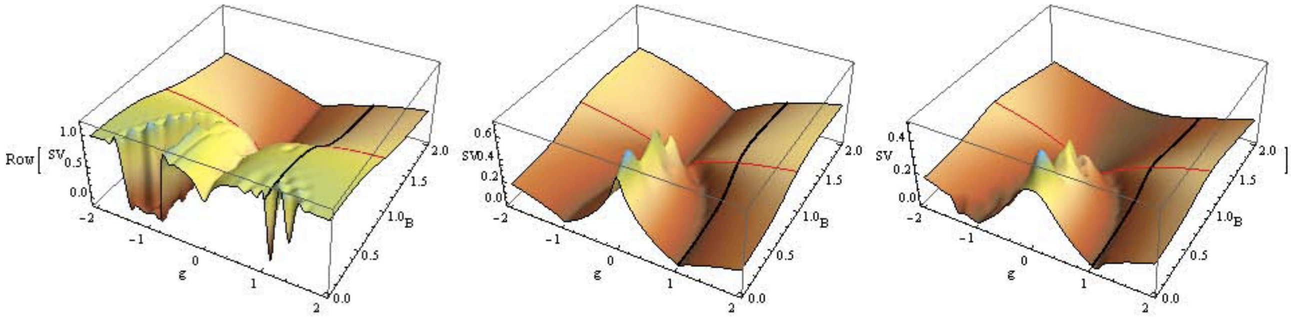

Fig.2. Singular values of the correlation matrix from the maximal (right plot) to minimal (left plot) for the ring of 16 spins.

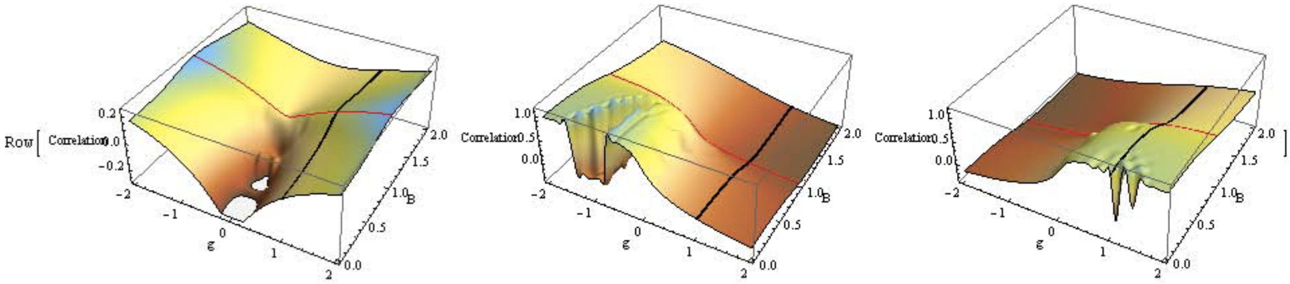

Fig.3. XX, YY and ZZ correlation functions from left to right.

Results for the magnetization M_x and M_z as a function of the parameters of the Hamiltonian is given on Fig. 4.

As we can see from this figures $M_z$magnetization for such a small system do not have a symmetry braking and essentially equals zero. M_x magnetization as it is expected grows with magnetic field ***B*** until system is fully magnetized.

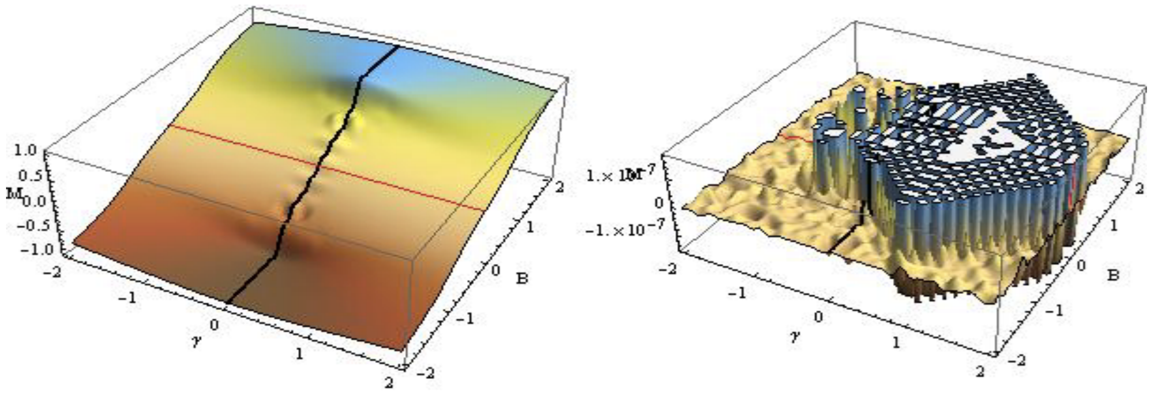

Fig.4. Magnetization as a function of the asymmetry and magnetic field for a 16 spins with open boundary conditions. Left: M_x. Right: M_z.

The interesting region for M_x magnetization, as we can see from Fig. 4, is at asymmetry value $\gamma = 0$. In this regime magnetization grows stepwise unless for the Ising case when $\gamma = 1$.

One can expect that increasing the number of sites in the quantum system magnetization at $\gamma = 0$ and $\gamma = 1$ shown on Fig. 4 will get closer and for the infinite system will coincide.

Another interesting results can be obtained introducing the explicit symmetry braking in the initial Hamiltonian that it takes the form of

$$H = \sum_{\{a,b\}\in\mathcal{B}} -\frac{1+\gamma}{2}\sigma_z^{(a)}\sigma_z^{(b)} - \frac{1-\gamma}{2}\sigma_y^{(a)}\sigma_y^{(b)} - \sum_{a\in V} \boldsymbol{B}\sigma_x^{(a)} - h\sigma_z^1$$

In this case magnetization M_z is not zero any more and shown on Fig. 5

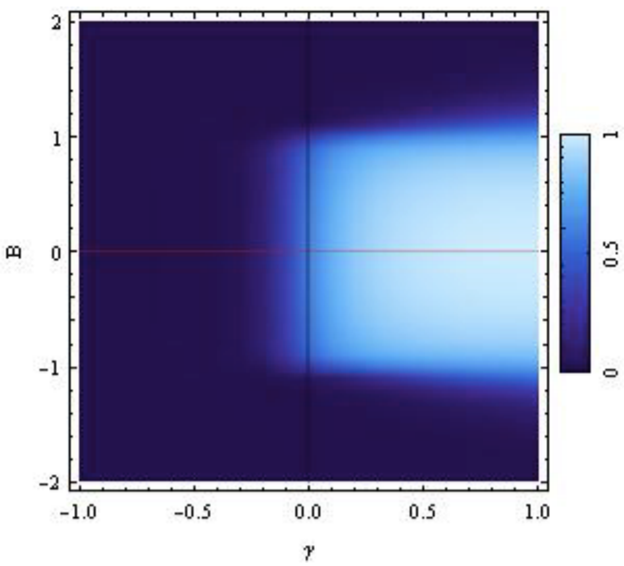

Fig.5. Magnetization M_z as a function of the $\boldsymbol{B}$ and γ for chain of $N = 16$ spins with symmetry braking.

The density plot of the M_z magnetization is given on the Fig. 5.

More clear the "classical" behavior of the M_z magnetization can be seen for the Ising model ($\gamma = 1$). This order parameter as a function of the magnetic field is given on Fig. 6.

As we can see the decay of the M_z magnetization become stronger if system is large. At thermodynamic limit $N \longrightarrow \infty$ the M_z is expected to vanish at the critical point $B = 1$.

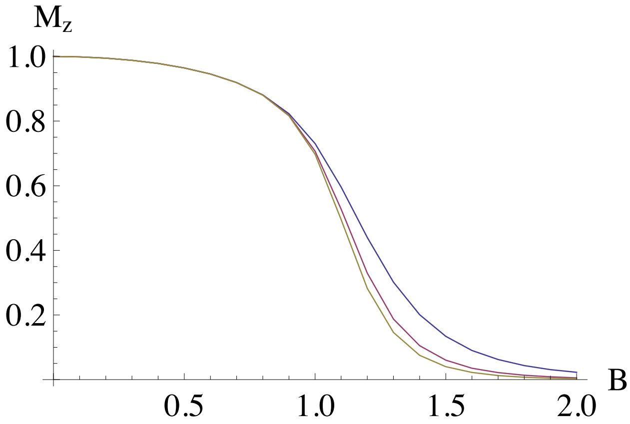

Fig.6. Magnetization M_z as a function of the $\boldsymbol{B}$ for $\gamma = 1$ (Ising) for chain of $N = 12$ (upper plot) $N = 16$ (middle plot) and $N = 18$ (lower plot) spins with symmetry braking.

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