Eigenvalues and eigenvectors of Ising model on hypercube

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Abstract. For a multidimensional Ising model, we expressed eigenvalues of the connection matrix in terms of the spin-spin interaction constants and trigonometric polynomials. In such systems, the eigenvectors are the Kronecker products of the well-known eigenvectors for the one-dimensional case. When boundary conditions are periodic, it is possible to obtain rigorous expressions for the eigenvalues when there is an arbitrary long-range interaction in the system.

1. Introduction

The Ising model is constantly in focus of the researcher’s attention. In part, this is due to its application when testing new methods for calculation of the free energy and critical characteristics. However, in spite of seeming simplicity, in some cases no exact solutions of this problem were found for about a hundred years [1] - [5].

In the present paper, we obtain rigorous expressions for eigenvalues of the connection matrices of Ising systems on hypercube. We examined the periodic boundary conditions supposing that each spin interacts with an arbitrary number of its neighbors. Up to now, the eigenvalues were known only in the special case of the nearest neighbor interaction [5].

In Section II, we present in detail our results for the one-dimensional Ising model. In this case, the form of matrices, which describe interactions of the given spin with its \( k \)-th neighbours (\( k = 1, 2, 3, \ldots \)) is very simple. Previously we showed that in the one-dimensional case these matrices commute [6]. This means that they all have the same set of eigenvectors. For one-dimensional lattices, this fact allows us to obtain the exact eigenvalues when the number of the interacting neighbours is arbitrary. We express the eigenvalues in terms of the spin-spin interaction constants and trigonometric polynomials. All the connection matrices have the same set of eigenvectors.

For one-dimensional systems, we solve the inverse problem. Namely, suppose we know an experimental energy spectrum of such a spin system (in other words, the set of the eigenvalues). We have to find out, what are the interactions it corresponds. This problem may have a practical interest.

In Section III, we outline briefly our results for two- and three-dimensional Ising models. For multidimensional problems, we express the eigenvalues of the connection matrices in terms of interaction constants between spins and the eigenvalues of the one-dimensional problem; the eigenvectors are the Kronecker products of the eigenvectors for the one-dimensional Ising system. Conclusions and discussion are in Section IV.

At the end of Introduction, we want to make some comments. In all the problems we discuss, the number of coordination spheres we take into account defines the number of interacting spins [7]. For a given lattice node, the \( k \)-th coordination sphere includes the nodes spaced from it by a distance occupying the \( k \)-th place in an increasing sequence of all different distances between the nodes. The
interactions between the nods belonging to the $k$-th coordination sphere and the given nod are the same. By $w_k$ we denote the relevant interaction constants. Note, for each problem we describe the interactions with an individual set $\{w_k\}$. Some constants $w_k$ can be equal to zero. This means that we do not account for such interactions.

When $k$ is not so large, there are traditional names for spins belonging to such coordination spheres: the nearest neighbors belong to the 1-st coordination sphere, the next neighbors belong to the 2-nd coordination sphere and the next-next neighbors belong to the 3-d coordination sphere. Somewhere in what follows, we will use this terminology.

2. One dimensional Ising model

Let us examine a one-dimensional Ising system that is a linear chain of $n$ connected spins $s_i = \pm 1$, where $i = 1, \ldots, n$.

In this case, the periodic boundary conditions mean that we transform the linear chain in a ring so that the $n$-th spin becomes the nearest neighbor of the first spin from “the left”, the $(n-1)$-th spin is the second (next) neighbor of the first spin, and so on (see Figure 1). It is easy to understand that for each spin the $k$-th coordination sphere includes two spins: the one that is spaced at $k$ spins to the right from the given spin and the spin that is at the same distance to the left.

Let $J(k)$ be a connection matrix of some one-dimensional Ising system when we account for the interactions with the spins of the $k$-th coordination sphere only. Then, for example, the matrices $J(1)$ and $J(2)$ are

$$J(1) = \begin{pmatrix} 0 & 1 & 0 & 0 & \ldots & 1 \\ 1 & 0 & 1 & 0 & \ldots & 0 \\ 0 & 1 & 0 & 1 & \ldots & 0 \\ \ldots & \ldots & \ldots & \ldots & \ldots & \ldots \\ 0 & 0 & \ldots & 1 & 0 & 1 \\ 1 & 0 & 0 & \ldots & 1 & 0 \end{pmatrix}, \quad J(2) = \begin{pmatrix} 0 & 0 & 1 & 0 & . & . & 1 \\ 0 & 0 & 0 & 1 & . & . & 1 \\ 1 & 0 & 0 & 0 & . & . & 0 \\ \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots \\ 1 & 0 & . & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & . & 1 & 0 & 0 \end{pmatrix}.$$}

Each matrix $J(k)$ is symmetric; it has the ones on its $k$-th and $(n-k)$-th superdiagonals, which are parallel to the main diagonal of the matrix. It is clear that $J(k) = J(n-k)$ and, consequently, the number of the coordination sphere is bounded from above: \(k \leq k_0 = \left\lfloor \frac{n}{2} \right\rfloor\). We use the matrices $\{J(k)\}_{k=1}^{k_0}$ to generate the connection matrix of the one-dimensional Ising system, where we account for interaction $w_i$ with the nearest neighbors, the interaction $w_2$ with the next neighbors, and so on:

$$H_i = w_1 \cdot J(1) + w_2 \cdot J(2) + \ldots + w_{k_0} \cdot J(k_0).$$

The formula (1) is rather general: it is valid for all possible interactions $w_k$ some of which may equal to zero.

With the aid of simple trigonometric calculations (see [6]), we can obtain the eigenvalues and eigenvectors of the matrix $J(1)$:

$$J(1) \cdot f_i = \lambda_i(1) \cdot f_i, \quad \text{where} \quad \lambda_i(1) = 2 \cdot \cos \varphi_i, \quad \varphi_i = \frac{2 \pi \cdot (i-1)}{n};$$

$$f_i = \left( f_i^{(1)}, \ldots, f_i^{(n)} \right)^t, \quad f_i^{(j)} = \frac{\cos(j-1)\varphi_i + \sin(j-1)\varphi_i}{\sqrt{n}}, \quad i, j = 1, 2, \ldots, n.$$
The first eigenvalue \( \lambda_1(1) = 2 \) is the largest and all the other eigenvalues \( \lambda_i(1) \) are double degenerate. Since the calculations for even and odd \( n \) differ slightly, in our discussion we suppose that \( n \) is odd. It is easy to see that the set of equalities

\[
\lambda_i(1) = \lambda_{n+2-i}(1), \quad i = 2, 3, \ldots, \frac{n+1}{2}.
\]

holds. In other words, if we do not account for the largest eigenvalue \( \lambda_1(1) = 2 \), the second half of the sequence of eigenvalues is a mirror image of the first half.

Let us use the matrix equality

\[
\mathbf{J}(k) \cdot \mathbf{J}(l) = \begin{cases} 
\mathbf{J}(k+l) + \mathbf{J}(k-l), & \text{when } k > l \\
\mathbf{J}(2k) + 2 \cdot \mathbf{I}, & \text{when } k = l 
\end{cases}
\]

where \( \mathbf{I} = \text{diag}(1,1,1) \) is a unit \((n \times n)\)-matrix. This equation allows us to show that the matrix \( \mathbf{J}(k) \) is a \( k \)-th degree polynomial of the matrix \( \mathbf{J}(1) \). Consequently, all these matrices commute and they all have the same set of eigenvectors \( \{ f_i \}^n_{i=1} \) (see Eq. (2)). This important quality is a basis of many following results.

With the aid of the above matrix equality, we can obtain the eigenvalues of the matrix \( \mathbf{J}(k) \):

\[
\lambda_i(k) = 2 \cdot \cos(k \cdot \varphi_i), \quad i = 1, 2, \ldots, n; \quad k = 1, 2, \ldots, k_0 = \left[ \frac{n}{2} \right].
\]

Note, the same as the eigenvalues of the matrix \( \mathbf{J}(1) \) (see Eq. (3)) the set of eigenvalues of each matrix \( \mathbf{J}(k) \) is mirror symmetric about the middle. We would like to recall that we do not take into account the largest eigenvalue \( \lambda_1(1) = 2 \).

Finally, equations (2) and (4) allow us to write the expression for the eigenvalues of the one-dimensional Ising connection matrix (1) in the most general form

\[
\lambda_i(\mathbf{H}_i) = w_i \cdot \lambda_1(1) + \ldots + w_{i_k} \lambda_i(k) = 2 \sum_{k=1}^{k_0} w_i \cdot \cos(k \cdot \varphi_i), \quad i = 1, 2, \ldots, n.
\]

The set \( \{ w_i \}^n_{i=1} \) define the interactions of the given spin with the spins from all the coordination spheres.

Suppose we know a dependence of the spin-spin interaction on the distance between the nodes of the lattice (for example, it may be \( w(r) = \exp(-f(r)) \) or \( w(r) = 1 / r^q \)), the it is possible to obtain an asymptotic expression for the spectral density of the one-dimensional Ising system.

Equation (5) allows us to make nontrivial conclusions about the general form of the spectrum of the one-dimensional Ising system. For example, it is clear that an arbitrary sequence of \( n \) numbers may be a spectrum only if it is mirror symmetric about the middle. We recall that we do not account for the largest eigenvalue \( \lambda_1(\mathbf{H}_i) \). Next, since there are zeros at the diagonal of the matrix \( \mathbf{J}(k) \) the equality

\[
\sum_{i=1}^{n} \lambda_i(k) = 0, \quad k = 1, 2, \ldots, k_0
\]

holds for each \( k \). With regard to Eq. (5), the same equality also holds for the spectrum of the one-dimensional Ising system. Then

\[
\sum_{i=1}^{n} \lambda_i(\mathbf{H}_i) = 0.
\]

Now we can formulate the conditions under which a sequence of arbitrary numbers \( \{ \lambda_i \}^n_{i=1} \) would be the spectrum of the one-dimensional Ising system. At first, it has to be mirror symmetric about the middle; in other words, the equality (3) must be fulfilled. The equality (6) defines the second (and the last) restriction. Namely, the sum of all the numbers \( \{ \lambda_i \}^n_{i=1} \) has to be equal to zero. From this requirement, we can find the value of the first term of the sequence:
\[ \lambda_i = -\sum_{i=2}^{n} \lambda_i = -2 \sum_{i=2}^{(n+1)/2} \lambda_i. \]  

(7)

As we see, with regard to equations (7) and (3) the \((n-1)/2\) numbers \(\lambda_2, \lambda_3, \ldots, \lambda_{(n+1)/2}\) define the spectrum of the one-dimension Ising system.

3. 2D and 3D Ising systems
In this Section, we will show our line of reasoning using as example a planar Ising model where we account for interactions with spins belonging to five nearest coordination spheres. In successive order, the first five distances between the lattice nodes are \(l_1 = 1\), \(l_2 = \sqrt{2}\), \(l_3 = 2\), \(l_4 = \sqrt{5}\), \(l_5 = 2\sqrt{2}\). In Figure 2, the circles denote the nodes, whose distances from the given node (the square in the lowest left angle of the figure) are equal to \(l_1\), \(l_2\), \(l_3\), \(l_4\), and \(l_5\), respectively. By \(\{w_k\}_i\) we denote the interaction constants with the spins of the corresponding coordination spheres.

![Figure 1. One dimensional Ising system.](image1)

![Figure 2. First five neighbors of the initial spin.](image2)

When generating a \((n^2 \times n^2)\)-connection matrix \(H_2\), we find that it has a block cyclic structure. “The building blocks” of the matrix \(H_2\) are \((n \times n)\)-matrices \(A_1, B_1, C_1, \ldots\) that are linear combinations of the matrices \(J(k)\) introduced in the previous Section. When we say that the matrix \(H_2\) is cyclic, we mean that each its subsequent block row is obtained by a cyclic shift of the previous row one position to the right. In the case under discussion the connection matrix has the form:

\[
\begin{pmatrix}
A_1 & B_1 & C_1 & 0 & \ldots & C_1 & B_1 \\
B_1 & A_1 & B_1 & C_1 & \ldots & 0 & C_1 \\
C_1 & B_1 & A_1 & B_1 & \ldots & 0 & 0 \\
0 & C_1 & B_1 & A_1 & \ldots & 0 & 0 \\
\vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\
C_1 & 0 & 0 & 0 & \ldots & A_1 & B_1 \\
B_1 & C_1 & 0 & 0 & \ldots & B_1 & A_1
\end{pmatrix}
\]

\(A_1 = w_1 J(1) + w_3 J(2),\)

where \(B_1 = w_1 I + w_2 J(1) + w_4 J(2),\)

\(C_1 = w_2 J + w_3 J(1) + w_5 J(2).\)

The eigenvectors of this matrix are the Kronecker products of the eigenvectors \(\{f_i\}_i\) for the one-dimensional problem (see Eq. (2)):

\[
F_{ij} = f_i \otimes f_j = \left( f_i^{(1)} f_j^{(1)} , f_i^{(1)} f_j^{(2)} , \ldots , f_i^{(1)} f_j^{(n)} , f_i^{(2)} f_j^{(1)} , f_i^{(2)} f_j^{(2)} , \ldots , f_i^{(2)} f_j^{(n)} , \ldots , f_i^{(n)} f_j^{(1)} , f_i^{(n)} f_j^{(2)} , \ldots , f_i^{(n)} f_j^{(n)} \right)^*.
\]

where \(i, j = 1, 2, \ldots , n.\)

We also may calculate the eigenvalues of the matrix \(H_2\). In the given case they are
\[ \mu_y = w_1 \left( \lambda_y(1) + \lambda_y(1) \right) + w_2 \lambda_y(1)\lambda_y(1) + w_3 \left( \lambda_y(2) + \lambda_y(2) \right) + w_4 \left( \lambda_y(1)\lambda_y(2) + \lambda_y(1)\lambda_y(2) \right) + w_5 \lambda_y(2)\lambda_y(2), \]

where \( \lambda_y(1) \) and \( \lambda_y(2) \) defined in equations (2) and (4).

In the same way we analyzed three-dimensional Ising model. The first step is to define the nodes belonging to the particular coordination spheres. The second step is to generate the connection matrix \( H_j \). The same as in the two-dimensional case it has a block cyclic structure but now “the building blocks” are \( (n^2 \times n^2) \)-matrices. The eigenvectors of the matrix \( H_j \) are the Kronecker products

\[ F_{ijk} = F_i \otimes F_j \otimes F_k, \]

where \( i, j, k = 1, 2, \ldots n \).

Let us write down the expression for the eigenvalues of the connection matrix \( H_j \) when we account for the interactions \( \{ w_i \}_{i=1}^5 \) with the five first coordination spheres:

\[ \mu_{ijk} = w_1 \left( \lambda_y(1) + \lambda_y(1) + \lambda_y(1) \right) + w_2 \left( \lambda_y(1)\lambda_y(1) + \lambda_y(1)\lambda_y(1) + \lambda_y(1)\lambda_y(1) \right) + w_3 \lambda_y(2)\lambda_y(1)\lambda_y(1) + \]
\[ + w_4 \left( \lambda_y(2) + \lambda_y(2) + \lambda_y(2) \right) + w_5 \left[ \left( \lambda_y(1) + \lambda_y(1) \right)\lambda_y(2) + \left( \lambda_y(1) + \lambda_y(1) \right)\lambda_y(2) + \left( \lambda_y(1) + \lambda_y(1) \right)\lambda_y(2) \right]. \]

The obtained exact expressions for the eigenvalues are the basis for examination of the spectral density of the multidimensional Ising systems.

4. Conclusions
In the present paper, we obtained analytical expressions for the eigenvalues of interaction matrices of Ising systems. We analyzed three lattices on hypercube of the dimensions: \( d = 1 \), \( d = 2 \), and \( d = 3 \). From our analysis, it follows that it is not difficult to generalize our results to the case of larger dimensions. Of special interest is the inverse problem, when it is necessary to define the interactions and the number of neighbours with which a spin interacts. This problem may be important for practical use.

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6. References
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