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The mathematical structure of the approximate linear response relation

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Abstract

In this paper, we study the mathematical structures of the linear response relation based on Plefka's expansion and the cluster variation method in terms of the perturbation expansion, and we show how this linear response relation approximates the correlation functions of the specified system. Moreover, by comparing the perturbation expansions of the correlation functions estimated by the linear response relation based on these approximation methods with exact perturbative forms of the correlation functions, we are able to explain why the approximate techniques using the linear response relation work well.

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1. Introduction

Random spin models are regarded as probabilistic models in which each pair of random variables interacts with each other. In this model, each node has a random variable (it is often called a spin variable), and some pairs of nodes are connected by links. These links represent interactions between random variables. In recent years, this kind of model and associated theories have been employed not only in statistical mechanics but also in some areas of information science [1, 2]. Since this kind of model has a complicated structure, using it for real applications requires reducing computational complexity. Mean-field theory (MFT) is a well-known theory to be used to avoid such problems. Thus, investigations of the MFT are important in information science as well as in statistical mechanics [1].

Plefka's expansion is one of the most important methods of the MFT [3]. Indeed, it is utilized to resolve problems in machine learning and other applications [2]. This method can be used to systematically obtain a perturbation from naive mean-field approximations and obtain the averages of each node with any order of approximation. Note that the average of

node means the average of the random variable at the node. Hence, the Thouless–Anderson–Palmer (TAP) equation [4, 5] and its higher-order approximations can be obtained within this method. The average of the node is one of the most basic and important variables in statistics. Therefore, Plefka's expansion is used for a wide range of problems. Besides the average of the node, the correlation function, or the covariant, is also an important variable in statistics. For instance, the correlation functions are employed in the learning algorithm of Boltzmann machines [6]. However, understanding how the correlation functions are calculated by using Plefka's expansion is nontrivial. Kappen and Rodríguez applied *the linear response relation* (LRR) to Plefka's expansion to calculate the correlation functions [7]. The correlation functions calculated by their method are approximate values, and it is well known that the accuracy is good [7–9]. The object of this work is to find why their method leads to good results. In order to investigate this, we need to examine the mathematical structure of the LRR based on Plefka's expansion.

The cluster variation method (CVM) is another one of the most important methods in the MFT [11]. In this method, the entropies of some of the sets of nodes are introduced such that one node entropies, two nodes entropies, etc, are regarded as the entropies of basic clusters. The entropy of a specified system is expressed approximately in terms of a linear combination of the entropies of these basic clusters. This method can be used to systematically obtain the mean-field and the Bethe approximations for a specified system. The CVM can treat the correlation functions within specified basic clusters, but the correlation functions between random variables on distant nodes are not taken into account directly in this method. Tanaka applied the LRR to the CVM and calculated the correlation functions between random variables on distant nodes and he showed that his method can quite accurately estimate such correlation functions in his numerical experiments [14]. Welling and Teh also applied the LRR to the Bethe approximation [13]. The Bethe approximation can estimate not only the averages of single nodes but also the correlation functions between random variables on neighboring pairs of nodes. In their numerical experiments, these authors compared the approximate accuracy of the correlation functions between random variables on neighboring pairs of nodes estimated by the LRR by using the Bethe approximation with those estimated only by the Bethe approximation and they concluded that the correlation functions estimated by the LRR based on the Bethe approximation are more precise than the other ones. In this paper, we are also interested in the mathematical structure of the LRR based on the CVM, and we want to find why it leads to good results.

Hence, the purpose of this paper is to examine the mathematical structure of the LRR based on Plefka's expansion and on the CVM to show why the LRR works well. In section 2, we outline Plefka's expansion and the approximate technique based on the LRR (we call this technique an approximate LRR in the present paper). In section 3, we show the exact form of the correlation functions using Plefka's expansion. In section 4, we see the mathematical structure of the LRR based on Plefka's expansion and compare it with the exact form given in section 3. In section 5, we consider the mathematical structure of the LRR based on the Bethe approximation and compare it with the exact form given in section 3. We provide some concluding remarks in section 6.

2. Plefka's expansion and the linear response theorem

Consider a graph consisting of N nodes. Each node is labeled by $i \in \{1, 2, \ldots, N\}$, and a binary random variable (or a spin variable) $S_i \in \{\pm 1\}$ is assigned to a node i, and some pair of the nodes are connected to each other by links. This system can be regarded as an Ising spin system. Each pair of nodes i and j interacts with each other by a weighted link which

is denoted by J_{ij}, and h_i acts on node i. Note that J_{ij} is symmetric for its index: $J_{ij} = J_{ji}$ and $J_{ii} = 0$. In statistical mechanics, these parameters $\{J_{ij}\}$ and $\{h_i\}$ are called *exchange interactions* and *external fields*, respectively. The Hamiltonian $\mathcal{H}$ determining energy for each configuration of random variables $\boldsymbol{S} = \{S_1, S_2, \ldots, S_N\}$ is given by

$$\mathcal{H}(\boldsymbol{S}, \boldsymbol{h}, \boldsymbol{J}) = -\sum_i h_i S_i - \sum_{(ij)} J_{ij} S_i S_j. \tag{1}$$

The summation in the first term of equation (1) is taken over all nodes and the summation in the second term of equation (1) is taken over all distinct pairs of nodes. The notation (ij) denotes the pair of nodes i and j. $\boldsymbol{h}$ and $\boldsymbol{J}$ denote a set of external fields h_i and exchange interactions J_{ij}, respectively; and they are given. The Helmholtz free energy for the system specified by the Hamiltonian $\mathcal{H}$ is

$$F(\boldsymbol{h}, \boldsymbol{J}, \beta) = -\frac{1}{\beta} \ln \sum_{\boldsymbol{S}} \exp\left(-\beta \mathcal{H}(\boldsymbol{S}, \boldsymbol{h}, \boldsymbol{J})\right), \tag{2}$$

where β is the inverse temperature and $\sum_{\boldsymbol{S}}$ denotes the summation taken over all configurations of random variables: $\sum_{\boldsymbol{S}} = \sum_{S_1=\pm 1} \sum_{S_2=\pm 1} \cdots \sum_{S_N=\pm 1}$. We want to calculate the averages of S_i at the thermal equilibrium state: $\langle S_i \rangle \equiv -\partial F(\boldsymbol{h}, \boldsymbol{J}, \beta)/\partial h_i = \sum_{\boldsymbol{S}} S_i\, p(\boldsymbol{S})$, where $\langle \cdot \rangle$ denotes the average with respect to the Boltzmann distribution of the Hamiltonian $\mathcal{H}$: $p(\boldsymbol{S}) \propto \exp\left(-\beta \mathcal{H}(\boldsymbol{S}, \boldsymbol{h}, \boldsymbol{J})\right)$. However, it is difficult to calculate these averages exactly because of computational complexity. Thus, we need to employ an approximation method.

2.1. Plefka's expansion

Plefka presented an effective method specifically for this kind of problem which is called *Plefka's expansion* [3] and that we now outline it briefly. Plefka introduced a parameter α into Hamiltonian (1) as follows:

$$\widehat{\mathcal{H}}(\boldsymbol{S}, \boldsymbol{h}, \boldsymbol{J}, \alpha) = -\sum_i h_i S_i - \alpha \sum_{(ij)} J_{ij} S_i S_j. \tag{3}$$

Then he introduced the Gibbs free energy G, which is obtained by the Legendre transform of the Helmholtz free energy determined by $\widehat{\mathcal{H}}$. Note that the Helmholtz free energy determined by $\widehat{\mathcal{H}}$ is

$$\widehat{F}(\boldsymbol{h}, \boldsymbol{J}, \beta, \alpha) = -\frac{1}{\beta} \ln \sum_{\boldsymbol{S}} \exp(-\beta \widehat{\mathcal{H}}(\boldsymbol{S}, \boldsymbol{h}, \boldsymbol{J}, \alpha)). \tag{4}$$

In the case of $\alpha = 1$, $\widehat{F} = F$ since $\widehat{\mathcal{H}} = \mathcal{H}$. And by defining m_i as $m_i \equiv -\partial \widehat{F}(\boldsymbol{h}, \boldsymbol{J}, \beta, \alpha)/\partial h_i$, the Gibbs free energy is obtained as follows:

$$G(\boldsymbol{m}, \boldsymbol{J}, \beta, \alpha) = \widehat{F}(\boldsymbol{h}, \boldsymbol{J}, \beta, \alpha) + \sum_i h_i(\boldsymbol{m}, \boldsymbol{J}, \beta, \alpha) m_i, \tag{5}$$

where $\boldsymbol{m} = \{m_1, m_2, \ldots, m_N\}$. This is the Legendre transform of the Helmholtz free energy in equation (4). Note that $\{m_i\}$ can be regarded as a set of independent variables, on which h_i depends on equation (5), i.e., $h_i = h_i(\boldsymbol{m}, \boldsymbol{J}, \beta, \alpha)$. It follows, then, that by expanding the Gibbs free energy G with respect to α, one gets the following series:

$$G(\boldsymbol{m}, \boldsymbol{J}, \beta, \alpha) = G(\boldsymbol{m}, \beta, 0) + \sum_{n=1}^{\infty} \frac{\alpha^n}{n!} g_n(\boldsymbol{m}, \boldsymbol{J}, \beta), \tag{6}$$

where for $n \geqslant 1$ we define

$$g_n(\boldsymbol{m}, \boldsymbol{J}, \beta) \equiv \left. \frac{\partial^n G(\boldsymbol{m}, \boldsymbol{J}, \beta, \alpha)}{\partial \alpha^n} \right|_{\alpha=0}. \tag{7}$$

This expansion is called Plefka's expansion. Since g_n is $\mathcal{O}(J_{ij}^n)$, this expansion can be regarded as the perturbation expansion with respect to weighted links $\{J_{ij}\}$. The coefficients of the expansion up to fourth order are given explicitly as follows [12, 15]:

$$G(\boldsymbol{m},\beta,0)=\frac{1}{\beta}\sum_i\left(\frac{1+m_i}{2}\ln\frac{1+m_i}{2}+\frac{1-m_i}{2}\ln\frac{1-m_i}{2}\right), \tag{8}$$

$$g_1(\boldsymbol{m},\boldsymbol{J},\beta)=-\sum_{(ij)}J_{ij}m_im_j, \tag{9}$$

$$g_2(\boldsymbol{m},\boldsymbol{J},\beta)=-\beta\sum_{(ij)}J_{ij}^2\left(1-m_i^2\right)\left(1-m_j^2\right), \tag{10}$$

$$\begin{aligned}g_3(\boldsymbol{m},\boldsymbol{J},\beta)=&-4\beta^2\sum_{(ij)}J_{ij}^3m_im_j\left(1-m_i^2\right)\left(1-m_j^2\right)\\&-6\beta^2\sum_{(ijk)}J_{ij}J_{jk}J_{ki}\left(1-m_i^2\right)\left(1-m_j^2\right)\left(1-m_k^2\right),\end{aligned} \tag{11}$$

$$\begin{aligned}g_4(\boldsymbol{m},\boldsymbol{J},\beta)=&-2\beta^3\sum_{(ij)}J_{ij}^4\left(1-m_i^2\right)\left(1-m_j^2\right)\left(15m_i^2m_j^2-3m_i^2-3m_j^2-1\right)\\&-48\beta^3\sum_{(ijk)}J_{ij}J_{jk}J_{ki}\left(1-m_i^2\right)\left(1-m_j^2\right)\left(1-m_k^2\right)\\&\times\left(J_{ij}m_im_j+J_{jk}m_jm_k+J_{ki}m_km_i\right)\\&-24\beta^3\sum_{(ijkl)}J_{ij}J_{jk}J_{kl}J_{li}\left(1-m_i^2\right)\left(1-m_j^2\right)\left(1-m_k^2\right)\left(1-m_l^2\right),\end{aligned} \tag{12}$$

where $\sum_{(ijk)}$ and $\sum_{(ijkl)}$ denote that the summation should be taken over all distinct 3- and 4-node clusters, respectively. By setting $\alpha=1$, the Hamiltonian $\widehat{\mathcal{H}}$ is equivalent to the original Hamiltonian $\mathcal{H}$, and equation (6) yields the true Gibbs free energy. Using one of the properties of the Legendre transform, i.e., $\partial G(\boldsymbol{m},\boldsymbol{J},\beta,\alpha)/\partial m_i=h_i(\boldsymbol{m},\boldsymbol{J},\beta,\alpha)$, one obtains self-consistent equations to determine $\{m_i\}$ at $\alpha=1$:

$$m_i=\tanh\beta\left(h_i+\sum_{n=1}^{\infty}\frac{1}{n!}\frac{\partial g_n(\boldsymbol{m},\boldsymbol{J},\beta)}{\partial m_i}\right). \tag{13}$$

Note that m_i determined by equation (13) is expected to be equal to the average of S_i: $m_i=\langle S_i\rangle$.

There are infinite terms in equation (6) thus, in practical, one approximates them by finite terms:

$$G(\boldsymbol{m},\boldsymbol{J},\beta,1)\approx G_n(\boldsymbol{m},\boldsymbol{J},\beta,1)=G(\boldsymbol{m},\beta,0)+\sum_{k=1}^{n}\frac{1}{k!}g_k(\boldsymbol{m},\boldsymbol{J},\beta), \tag{14}$$

where $G_n(\boldsymbol{m},\boldsymbol{J},\beta,1)$ is the nth-order approximation of $G(\boldsymbol{m},\boldsymbol{J},\beta,1)$. Since g_n is $\mathcal{O}(J_{ij}^n)$, G_n is regarded as an approximation neglecting terms of $\mathcal{O}(J_{ij}^{n+1})$ in the true Gibbs free energy. Under this approximation, $\{m_i\}$ are determined by the following self-consistent equations:

$$m_i=\tanh\beta\left(h_i+\sum_{k=1}^{n}\frac{1}{k!}\frac{\partial g_k(\boldsymbol{m},\boldsymbol{J},\beta)}{\partial m_i}\right). \tag{15}$$

One regards m_i determined by equation (15) as the nth-order approximation of $\langle S_i\rangle$.

For instance, the first-order approximation specified by G_1 leads to the naive mean-field approximation, and the second-order approximation specified by G_2 leads to the TAP approximation. Hence, Plefka's expansion can systematically derive the mean-field, the TAP or higher-order approximations of the system [3, 12, 15].

2.2. *The approximate LRR*

In the framework of Plefka's expansion, one can calculate the average of the random variables of the system with any order of approximation. However, it is nontrivial to consider how the correlation functions $\langle S_i S_j \rangle$ are obtained within this framework. Kappen and several authors calculated the correlation functions approximately by applying the LRR to Plefka's expansion [7–9]. The differentiation of the Helmholtz free energy in equation (2) with respect to h_i and h_j is

$$\frac{\partial^2 F(\boldsymbol{h}, \boldsymbol{J}, \beta)}{\partial h_i \partial h_i} = -\beta \left(\langle S_i S_j \rangle - \langle S_i \rangle \langle S_j \rangle \right) \equiv -\chi_{ij}. \tag{16}$$

We now introduce the matrices $\boldsymbol{\chi}$ and $\boldsymbol{A}$ whose elements ij are χ_{ij} and A_{ij}, respectively. A_{ij} is defined by

$$A_{ij} \equiv \frac{\partial^2 G(\boldsymbol{m}, \boldsymbol{J}, \beta, 1)}{\partial m_i \partial m_j}. \tag{17}$$

The matrices $\boldsymbol{\chi}$ and $\boldsymbol{A}$ are each other's inverse, i.e., $\boldsymbol{\chi} = \boldsymbol{A}^{-1}$. This is the property of the Legendre transform [7, 8]. Therefore, one can calculate a correlation function $\langle S_i S_j \rangle$ by the relation

$$\langle S_i S_j \rangle = \frac{1}{\beta} \chi_{ij} + \langle S_i \rangle \langle S_j \rangle = \frac{1}{\beta} [\boldsymbol{A}^{-1}]_{ij} + m_i m_j, \tag{18}$$

where $[\boldsymbol{A}^{-1}]_{ij}$ is the element ij of the inverse of the matrix $\boldsymbol{A}$ and $\{m_i\}$ are determined by equation (13). If one considers all the terms in equation (6), the last equality in equation (18) is true. The relationship expressed by equation (18) is known as the LRR.

To obtain the correlation functions approximately, the matrix $\boldsymbol{A}$ is replaced by the matrix $\boldsymbol{A}^{(n)}$, whose element ij is defined by

$$A_{ij}^{(n)} \equiv \frac{\partial^2 G_n(\boldsymbol{m}, \boldsymbol{J}, \beta, 1)}{\partial m_i \partial m_j}, \tag{19}$$

where $G_n(\boldsymbol{m}, \boldsymbol{J}, \beta, 1)$ is the nth-order approximation of $G(\boldsymbol{m}, \boldsymbol{J}, \beta, 1)$. Thus, one obtains $m_{ij}^{(n)}$, which is the nth-order approximation of the correlation function by using the LRR, defined by

$$m_{ij}^{(n)} \equiv \frac{1}{\beta} \chi_{ij}^{(n)} + m_i m_j, \tag{20}$$

where $\chi_{ij}^{(n)}$ is the element ij of the matrix $\boldsymbol{\chi}^{(n)}$, which is the inverse of the matrix $\boldsymbol{A}^{(n)}$, i.e., $\boldsymbol{\chi}^{(n)} = (\boldsymbol{A}^{(n)})^{-1}$, and $\{m_i\}$ are determined by equation (15). To distinguish equation (20) from equation (18), we call equation (20) an *approximate LRR*. Although the approximate LRR does not hold exactly, it can be assumed to hold approximately: $\langle S_i S_j \rangle \approx m_{ij}^{(n)}$. However, it is not clear how equation (20) approximates true correlation functions.

3. Exact expanded form of correlation functions

In this section, we show the exact perturbative form of the correlation functions using Plefka's expansion as given in section 2. The parameters $\{J_{ij}\}$ are independent variables of both $\widehat{F}(\boldsymbol{h}, \boldsymbol{J}, \beta, \alpha)$ and $G(\boldsymbol{m}, \boldsymbol{J}, \beta, \alpha)$, and both are the Legendre transform of each other. It is the basic property of the Legendre transform that the derivatives of $\widehat{F}(\boldsymbol{h}, \boldsymbol{J}, \beta, \alpha)$ and $G(\boldsymbol{m}, \boldsymbol{J}, \beta, \alpha)$ with respect to such kind of variables as $\{J_{ij}\}$ (sometimes these variables are called *passive variables*) are equivalent. In fact, this property is confirmed easily by differentiating equation (5) with respect to J_{ij}:

$$\begin{aligned}\frac{\partial G(\boldsymbol{m}, \boldsymbol{J}, \beta, \alpha)}{\partial J_{ij}} &= \frac{\partial \widehat{F}(\boldsymbol{h}, \boldsymbol{J}, \beta, \alpha)}{\partial J_{ij}} + \sum_k \frac{\partial \widehat{F}(\boldsymbol{h}, \boldsymbol{J}, \beta, \alpha)}{\partial h_k}\frac{\partial h_k}{\partial J_{ij}} + \sum_k \frac{\partial h_k}{\partial J_{ij}} m_k \\ &= \frac{\partial \widehat{F}(\boldsymbol{h}, \boldsymbol{J}, \beta, \alpha)}{\partial J_{ij}}, \end{aligned} \tag{21}$$

where we use the relation $m_i = -\partial \widehat{F}(\boldsymbol{h}, \boldsymbol{J}, \beta, \alpha)/\partial h_i$. This equation holds for any value of α. Thus, setting $\alpha = 1$, we obtain

$$\frac{\partial F(\boldsymbol{h}, \boldsymbol{J}, \beta)}{\partial J_{ij}} = \frac{\partial G(\boldsymbol{m}, \boldsymbol{J}, \beta, 1)}{\partial J_{ij}}. \tag{22}$$

Since $\partial F(\boldsymbol{h}, \boldsymbol{J}, \beta)/\partial J_{ij} = -\langle S_i S_j \rangle$, using equation (6), equation (22) yields

$$\begin{aligned}\langle S_i S_j \rangle &= -\frac{\partial}{\partial J_{ij}} G(\boldsymbol{m}, \beta, 0) - \frac{\partial}{\partial J_{ij}} \sum_{n=1}^{\infty} \frac{1}{n!} g_n(\boldsymbol{m}, \boldsymbol{J}, \beta) \\ &= -\frac{\partial}{\partial J_{ij}} \sum_{n=1}^{\infty} \frac{1}{n!} g_n(\boldsymbol{m}, \boldsymbol{J}, \beta). \end{aligned} \tag{23}$$

This is the exact expanded form of the correlation functions. Using equations (23) and (9)–(12), we can express the explicit form of the present expansion as follows:

$$\begin{aligned}\langle S_i S_j \rangle = {} & m_i m_j + \beta J_{ij}\left(1 - m_i^2\right)\left(1 - m_j^2\right) + 2\beta^2 J_{ij}^2 m_i m_j \left(1 - m_i^2\right)\left(1 - m_j^2\right) \\ & + \beta^2 \left(1 - m_i^2\right)\left(1 - m_j^2\right) \sum_k J_{jk} J_{ki} \left(1 - m_k^2\right) \\ & + \frac{\beta^3 J_{ij}^3}{3}\left(1 - m_i^2\right)\left(1 - m_j^2\right)\left(15 m_i^2 m_j^2 - 3m_i^2 - 3m_j^2 - 1\right) \\ & + 4\beta^3 J_{ij} m_i m_j \left(1 - m_i^2\right)\left(1 - m_j^2\right) \sum_k J_{jk} J_{ki} \left(1 - m_k^2\right) \\ & + 2\beta^3 \left(1 - m_i^2\right)\left(1 - m_j^2\right) \sum_k J_{jk} J_{ki} m_k \left(1 - m_k^2\right)\left(J_{jk} m_j + J_{ki} m_i\right) \\ & + \beta^3 \left(1 - m_i^2\right)\left(1 - m_j^2\right) \sum_{k \neq i} \sum_{l \neq j} J_{jk} J_{kl} J_{li} \left(1 - m_k^2\right)\left(1 - m_l^2\right) + \mathcal{O}\left(J_{ij}^4\right), \end{aligned} \tag{24}$$

where $\{m_i\}$ are determined by equation (13), i.e., $m_i = \langle S_i \rangle$. The summation $\sum_{k \neq i}$ refers to the summation taken over all the nodes except node i.

If there is no link between nodes i and j, the correlation function between random variables S_i and S_j is

$$\begin{aligned}\langle S_i S_j\rangle = {} & m_i m_j + \beta^2\left(1-m_i^2\right)\left(1-m_j^2\right)\sum_k J_{jk}J_{ki}\left(1-m_k^2\right) \\ & + 2\beta^3\left(1-m_i^2\right)\left(1-m_j^2\right)\sum_k J_{jk}J_{ki}m_k\left(1-m_k^2\right)\left(J_{jk}m_j + J_{ki}m_i\right) \\ & + \beta^3\left(1-m_i^2\right)\left(1-m_j^2\right)\sum_{k\neq i}\sum_{l\neq j} J_{jk}J_{kl}J_{li}\left(1-m_k^2\right)\left(1-m_l^2\right) + \mathcal{O}\left(J_{ij}^4\right), \end{aligned} \tag{25}$$

which can be obtained by setting $J_{ij} = 0$ in equation (24). Equation (25) expresses the dependence between non-connecting nodes.

The framework of the (approximate) LRR is widely employed to calculate correlations in several scientific areas besides physics [10]. However, the exact series expression of the correlation functions on each system is not always obtained specifically as in this section. Therefore, to clarify the property of the approximate LRR analytically, we suggest that it is important to compare the correlation functions estimated by the approximate LRR with the exact series expression of the correlation functions where their exact series expression can be obtained specifically. Thus, in the following section, we will examine the mathematical structures of the approximate LRR expressed by equation (20) in terms of the perturbation expansion and will compare them with equation (24).

4. The mathematical structure of the approximate LRR

In this section, we examine the mathematical structures of the approximate LRR in terms of the perturbation expansion with respect to weighted links J_{ij} and clarify the reasons why the approximate LRR in equation (20) can be expected to be a good approximation of the correlation functions. We expand the right-hand side of equation (20) at $n = 1$ and $n = 2$ with respect to weighted links J_{ij} and compare them with the exact form in equation (24).

4.1. The first-order approximation of the approximate LRR

The correlation function using the first-order approximation of the approximate LRR is

$$m_{ij}^{(1)} = \frac{1}{\beta}\chi_{ij}^{(1)} + m_i m_j, \tag{26}$$

where $\{m_i\}$ are determined by equation (15) with $n = 1$; that is to say, the naive mean-field equation. Since

$$A_{ij}^{(1)} = \frac{\partial^2 G_1(\boldsymbol{m}, \boldsymbol{J}, \beta, 1)}{\partial m_i \partial m_j} = \frac{\delta_{ij}}{\beta\left(1-m_i^2\right)} - J_{ij}, \tag{27}$$

$\chi_{ij}^{(1)}$, which is the element ij of the matrix $\boldsymbol{\chi}^{(1)}$, is expanded as follows:

$$\begin{aligned}\chi_{ij}^{(1)} = {} & \beta^2 J_{ij}\left(1-m_i^2\right)\left(1-m_j^2\right) + \beta^3\left(1-m_i^2\right)\left(1-m_j^2\right)\sum_k J_{jk}J_{ki}\left(1-m_k^2\right) \\ & + \beta^4\left(1-m_i^2\right)\left(1-m_j^2\right)\sum_k\sum_l J_{jk}J_{kl}J_{li}\left(1-m_k^2\right)\left(1-m_l^2\right) + \mathcal{O}\left(J_{ij}^4\right), \end{aligned} \tag{28}$$

where $i \neq j$, and

$$\chi_{ii}^{(1)} = \beta\left(1-m_i^2\right) + \beta^3\left(1-m_i^2\right)^2 \sum_j J_{ij}^2\left(1-m_j^2\right) + \beta^4\left(1-m_i^2\right)^2 \sum_j \sum_k J_{ij}J_{jk}J_{ki}\left(1-m_j^2\right)\left(1-m_k^2\right) + \mathcal{O}\left(J_{ij}^4\right). \tag{29}$$

From equations (26), (28) and (29) the correlation function using the first-order approximation of the approximate LRR yields

$$m_{ij}^{(1)} = m_i m_j + \beta J_{ij}\left(1-m_i^2\right)\left(1-m_j^2\right) + \beta^2\left(1-m_i^2\right)\left(1-m_j^2\right)\sum_k J_{jk}J_{ki}\left(1-m_k^2\right) + \beta^3\left(1-m_i^2\right)\left(1-m_j^2\right)\sum_k \sum_l J_{jk}J_{kl}J_{li}\left(1-m_k^2\right)\left(1-m_l^2\right) + \mathcal{O}\left(J_{ij}^4\right) \tag{30}$$

and

$$\begin{aligned} m_{ii}^{(1)} &= 1 + \beta^2\left(1-m_i^2\right)^2 \sum_j J_{ij}^2\left(1-m_j^2\right) \\ &\quad + \beta^3\left(1-m_i^2\right)^2 \sum_j \sum_k J_{ij}J_{jk}J_{ki}\left(1-m_j^2\right)\left(1-m_k^2\right) + \mathcal{O}\left(J_{ij}^4\right) \\ &= 1 + \mathcal{O}\left(J_{ij}^2\right). \end{aligned} \tag{31}$$

When comparing equation (24) with equation (30), we immediately find that up to the first-order terms both have the same form. It can be explained as follows: $G_1(\boldsymbol{m}, \boldsymbol{J}, \beta, 1)$ can be identified with $G(\boldsymbol{m}, \boldsymbol{J}, \beta, 1)$ in a system where the terms of $\mathcal{O}\left(J_{ij}^2\right)$ can be neglected because, in such a case, $A_{ij}^{(1)} = A_{ij}$, $\chi_{ij}^{(1)} = \chi_{ij}$. From equation (24), $\langle S_i S_j \rangle = m_i m_j + \beta J_{ij}\left(1-m_i^2\right)\left(1-m_j^2\right) + \mathcal{O}\left(J_{ij}^2\right)$ and, therefore, the correlation function obtained by using the first-order approximation of the approximate LRR must be $m_{ij}^{(1)} = m_i m_j + \beta J_{ij}\left(1-m_i^2\right)\left(1-m_j^2\right) + \mathcal{O}\left(J_{ij}^2\right)$.

It should be noted that $m_{ij}^{(1)}$ has some contributions of the higher-order terms in equation (24). Although G_1 neglects the contribution of the terms of $\mathcal{O}\left(J_{ij}^2\right)$, $m_{ij}^{(1)}$ includes partial higher-order terms higher than the terms of $\mathcal{O}(J_{ij})$ in equation (24) (compare equations (24) with (30)). Indeed, the third term of equation (30) corresponds to the fourth term of equation (24), and the fourth term of equation (30) includes the eighth term of equation (24). This suggests that some higher-order terms in $m_{ij}^{(1)}$ originate from the lower-order terms in G_1. This is an important characteristic of the approximate LRR. Although we expect that $m_{ii}^{(1)} \approx \langle S_i^2 \rangle = 1$, $m_{ii}^{(1)}$ generally differs from 1 by the contribution of the terms of $\mathcal{O}\left(J_{ij}^2\right)$.

In the case of this approximation, we can calculate the general terms of $m_{ij}^{(1)}$, and the result is as follows (see appendix A):

$$m_{ij}^{(1)} = m_i m_j + \beta J_{ij}\left(1-m_i^2\right)\left(1-m_j^2\right) + \left(1-m_i^2\right)\left(1-m_j^2\right)\sum_{n=1}^{\infty} \beta^{n+1} \sum_{i_1, i_2, \ldots, i_n} J_{ii_1}J_{i_1i_2}\cdots J_{i_nj} \times \left(1-m_{i_1}^2\right)\left(1-m_{i_2}^2\right)\cdots\left(1-m_{i_n}^2\right). \tag{32}$$

This correlation function includes the contribution of the terms which are dominant in the case of the Hopfield model [15], and these terms can be expected to appear among the higher-order terms in equation (24).

Since it is difficult to estimate the contribution of the higher order terms of $m_{ij}^{(1)}$ for general cases, as an example, we will explain it briefly with the simple case as follows. We consider the system where all pair of nodes are connected, i.e., the full-connected graph, and all J_{ij}'s

and h_i's take the constant values: $J_{ij} = J/N$ and $h_i = h$. It is one of the simplest *mean-field models*. From uniformity of the system, averages $\langle S_i \rangle$ for all i should take the same value and, thus, we write $\langle S_i \rangle \equiv \langle S \rangle$ for all i. Moreover, m_i for all i determined by the naive mean-field equations should also take the same value and, thus, we write $m_i \equiv m$ for all i. In this case, for large N, $\langle S_i S_j \rangle$ in equation (24) obtained by Plefka's expansion and $m_{ij}^{(1)}$ in equation (30) obtained by the approximate LRR up to the presented orders are reduced to

$$\begin{aligned}\langle S_i S_j \rangle = \langle S \rangle^2 &+ \frac{\beta J}{N}(1 - \langle S \rangle^2)^2 + \frac{2\beta^2 J^2}{N^2}\langle S \rangle^2 (1 - \langle S \rangle^2)^2 + \frac{\beta^2 J^2}{N}(1 - \langle S \rangle^2)^3 \\ &+ \frac{\beta^3 J^3}{3N^3}(1 - \langle S \rangle^2)^2 (15\langle S \rangle^4 - 6\langle S \rangle^2 - 1) + \frac{8\beta^3 J^3}{N^2}\langle S \rangle^2 (1 - \langle S \rangle^2)^3 \\ &+ \frac{\beta^3 J^3}{N}(1 - \langle S \rangle^2)^4 + \mathcal{O}(\beta^4 J^4) \end{aligned} \tag{33}$$

and

$$m_{ij}^{(1)} = m^2 + \frac{\beta J}{N}(1 - m^2)^2 + \frac{\beta^2 J^2}{N}(1 - m^2)^3 + \frac{\beta^3 J^3}{N}(1 - m^2)^4 + \mathcal{O}(\beta^4 J^4), \tag{34}$$

respectively. When comparing equations (33) and (34), we find that $m_{ij}^{(1)}$ includes the contribution of only the terms of $\mathcal{O}(1)$ and $\mathcal{O}(1/N)$ in equation (33), and omits those of $\mathcal{O}(1/N^2)$ therein. Except the terms of $\mathcal{O}(1)$, i.e., the first terms of equations (33) and (34), the terms of $\mathcal{O}(1/N)$ are the most dominant and are expected to play an important role for large N. This simple example suggests that $m_{ij}^{(1)}$ treats the significant terms effectively. This argument is not always valid in general cases, but we think that the situation is similar for the systems where variances of the distribution of the external interactions are small.

Diagonal elements of the approximate LRR, $m_{ii}^{(1)}$ in equation (31), up to the presented order are reduced to

$$m_{ii}^{(1)} = 1 + \frac{\beta^2 J^2}{N}(1 - m^2)^3 + \frac{\beta^3 J^3}{N}(1 - m^2)^4 + \mathcal{O}(\beta^4 J^4), \tag{35}$$

for the above simple system. If the difference between $\langle S \rangle$ and m is very small, the terms of $\mathcal{O}(1)$ and $\mathcal{O}(1/N)$ in equation (34) are almost corresponding to those in equation (33). Therefore, $m_{ij}^{(1)}$ is almost corresponding to $\langle S_i S_j \rangle$ up to $\mathcal{O}(1/N)$ in high-temperature regions. While, the difference between 1 and $m_{ii}^{(1)}$ keeps $\mathcal{O}(1/N)$ at any m within $(-1, 1)$. It may be said that the approximation of $\langle S_i S_j \rangle$ and $\langle S_i^2 \rangle (= 1)$ is qualitatively different in the presented method. Identifying the reason why such a difference arises is one of our future objectives.

4.2. The second-order approximation of the approximate LRR

The correlation function using the second-order approximation of the approximate LRR is

$$m_{ij}^{(2)} = \frac{1}{\beta}\chi_{ij}^{(2)} + m_i m_j, \tag{36}$$

where $\{m_i\}$ are determined by equation (15) with $n = 2$, which is the TAP equation. Since

$$\begin{aligned} A_{ij}^{(2)} &= \frac{\partial^2}{\partial m_i \partial m_j} G_2(\boldsymbol{m}, \boldsymbol{J}, \beta, 1) \\ &= \left\{ \frac{1}{\beta\left(1 - m_i^2\right)} - J_{ij} + \beta \sum_k J_{ik}\left(1 - m_k^2\right) \right\} \delta_{ij} - J_{ij} - 2\beta J_{ij}^2 m_i m_j, \end{aligned} \tag{37}$$

by expanding $\chi_{ij}^{(2)}$, which is the element ij of the matrix $\boldsymbol{\chi}^{(2)}$ defined as the inverse of the matrix $\boldsymbol{A}^{(2)}$, in a similar way to the previous section and using equation (36), we obtain the correlation function when using the second-order approximation of the approximate LRR as follows:

$$\begin{aligned} m_{ij}^{(2)} = {} & m_i m_j + \beta J_{ij}\left(1-m_i^2\right)\left(1-m_j^2\right) + 2\beta^2 J_{ij}^2 m_i m_j \left(1-m_i^2\right)\left(1-m_j^2\right) \\ & + \beta^2\left(1-m_i^2\right)\left(1-m_j^2\right)\sum_k J_{jk}J_{ki}\left(1-m_k^2\right) \\ & + 2\beta^3\left(1-m_i^2\right)\left(1-m_j^2\right)\sum_k J_{jk}J_{ki}m_k\left(1-m_k^2\right)\left(J_{jk}m_j + J_{ki}m_i\right) \\ & + \beta^3\left(1-m_i^2\right)\left(1-m_j^2\right)\sum_{k\neq i}\sum_{l\neq j} J_{jk}J_{kl}J_{li}\left(1-m_k^2\right)\left(1-m_l^2\right) \\ & - \beta^3 J_{ij}^3\left(1-m_i^2\right)^2\left(1-m_j^2\right)^2 + \mathcal{O}\left(J_{ij}^4\right) \end{aligned} \tag{38}$$

and

$$\begin{aligned} m_{ii}^{(2)} = {} & 1 + \beta^3\left(1-m_i^2\right)^2 \sum_{j\neq i}\sum_{k\neq i} J_{ij}J_{jk}J_{ki}\left(1-m_j^2\right)\left(1-m_k^2\right) \\ & + 4\beta^3 m_i\left(1-m_i^2\right)^2 \sum_j J_{ij}^3 m_j\left(1-m_j^2\right) + \mathcal{O}\left(J_{ij}^4\right) \\ = {} & 1 + \mathcal{O}\left(J_{ij}^3\right). \end{aligned} \tag{39}$$

A comparison of equations (24) with (38) shows that up to the second-order both have the same form, and $m_{ij}^{(2)}$ has contributions of some higher-order terms than $\mathcal{O}\left(J_{ij}^2\right)$ in equation (24) (compare equations (24) with (38)). $m_{ij}^{(2)}$ takes the contributions of higher-order terms in equation (24) into account more precise than $m_{ij}^{(1)}$. Therefore, $m_{ij}^{(2)}$ can be expected to accommodate complex situations better than $m_{ij}^{(1)}$. Moreover, from equation (39), $m_{ii}^{(2)}$ is not equal to 1 as a result of the contribution of the terms of $\mathcal{O}\left(J_{ij}^3\right)$.

From the above arguments presented in this section, we found that the correlation functions estimated by the approximate LRR have contributions of some higher-order terms than terms taken into account in G_n. For instance, in spite of neglecting the terms of $\mathcal{O}\left(J_{ij}^2\right)$ in G_1, $m_{ij}^{(1)}$, which is calculated by using G_1, has contributions of some of the terms of $\mathcal{O}\left(J_{ij}^2\right)$ in equation (24). Similarly, in spite of neglecting terms of $\mathcal{O}\left(J_{ij}^3\right)$ in G_2, $m_{ij}^{(2)}$, which is calculated by using G_2, has contributions of some of the terms of $\mathcal{O}\left(J_{ij}^3\right)$ in equation (24). It is an important property of the approximate LRR. This property is the reason why the approximate LRR can be assumed to be a good approximation of the correlation functions.

5. Correlation functions estimated by the Bethe approximation and by the approximate LRR

In this section, we compare the correlation functions estimated by the Bethe approximation in the CVM with those obtained by the approximate LRR. The Bethe approximation can estimate not only the average of the random variables on each of the nodes but also the correlation functions between two distinct random variables on each neighboring pair of nodes. The Bethe approximation regards the correlation function between S_i and S_j as

$$\xi_{ij} = \coth(2\beta J_{ij})\left(1 - \sqrt{1 - \left(1 - {m_i}^2 - {m_j}^2\right)\tanh^2(2\beta J_{ij}) - 2m_i m_j \tanh(2\beta J_{ij})}\right), \tag{40}$$

where ξ_{ij} denotes the correlation function estimated by the Bethe approximation, and $\{m_i\}$ are determined by the Bethe approximation [16]. It is well known that the Bethe approximation gives exact results when the system is regarded as a tree. By expanding ξ_{ij} with respect to J_{ij}, we obtain the following series:

$$\xi_{ij} = m_i m_j + \beta J_{ij}\left(1-m_i^2\right)\left(1-m_j^2\right) + 2\beta^2 J_{ij}^2 m_i m_j \left(1-m_i^2\right)\left(1-m_j^2\right) + \frac{\beta^3 J_{ij}^3}{3}\left(1-m_i^2\right)\left(1-m_j^2\right)\left(15m_i^2 m_j^2 - 3m_i^2 - 3m_j^2 - 1\right) + \mathcal{O}\left(J_{ij}^4\right). \tag{41}$$

It is known that the Bethe–Gibbs free energy includes only the contributions of the mean-field entropies and the contributions of neighboring pair of nodes in Plefka's expansion (equations (8)–(10) and the first term of equations (11) and (12)) [16]. Thus, the Bethe–Gibbs free energy is

$$G_B(\boldsymbol{m}, \boldsymbol{J}, \beta) = \frac{1}{\beta}\sum_i \left(\frac{1+m_i}{2}\ln\frac{1+m_i}{2} + \frac{1-m_i}{2}\ln\frac{1-m_i}{2}\right) - \sum_{(ij)} J_{ij} m_i m_j - \frac{\beta}{2}\sum_{(ij)} J_{ij}^2\left(1-m_i^2\right)\left(1-m_j^2\right) - \frac{2\beta^2}{3}\sum_{(ij)} J_{ij}^3 m_i m_j \left(1-m_i^2\right)\left(1-m_j^2\right) - \frac{\beta^3}{12}\sum_{(ij)} J_{ij}^4\left(1-m_i^2\right)\left(1-m_j^2\right)\left(15m_i^2 m_j^2 - 3m_i^2 - 3m_j^2 - 1\right) + \mathcal{O}\left(J_{ij}^5\right). \tag{42}$$

The explicit derivation of G_B in equation (42) is given in appendix B.

To apply the framework of the approximate LRR in equation (20) to equation (42), it is possible to express the correlation function as

$$m_{ij}^{(B)} = \frac{1}{\beta}\chi_{ij}^{(B)} + m_i m_j, \tag{43}$$

where $m_{ij}^{(B)}$ denotes the correlation function estimated by the approximate LRR based on the Bethe approximation and $\chi_{ij}^{(B)}$ denotes element ij of a matrix which is the inverse of the matrix $\boldsymbol{A}^{(B)}$, whose element ij is defined by

$$A_{ij}^{(B)} \equiv \frac{\partial^2}{\partial m_i \partial m_j} G_B(\boldsymbol{m}, \boldsymbol{J}, \beta) = \left\{\frac{1}{\beta\left(1-m_i^2\right)} + \beta\sum_k J_{ik}^2\left(1-m_k^2\right) + 4\beta^2\sum_k J_{ik}^3 m_i m_k (1-m_k)^2\right\}\delta_{ij} - J_{ij} - 2\beta J_{ij}^2 m_i m_j - \frac{2\beta^2 J_{ij}^3}{3}\left(1-3m_i^2\right)\left(1-3m_j^2\right) + \mathcal{O}\left(J_{ij}^4\right). \tag{44}$$

Expanding $\chi_{ij}^{(B)}$ with respect to the weighted links $\{J_{ij}\}$ and using equation (43), we obtain

$$m_{ij}^{(B)} = m_i m_j + \beta J_{ij}\left(1-m_i^2\right)\left(1-m_j^2\right) + 2\beta^2 J_{ij}^2 m_i m_j \left(1-m_i^2\right)\left(1-m_j^2\right) + \beta^2\left(1-m_i^2\right)\left(1-m_j^2\right)\sum_k J_{ik} J_{kj}\left(1-m_k^2\right) + \frac{\beta^3 J_{ij}^3}{3}\left(1-m_i^2\right)\left(1-m_j^2\right)\left(15m_i^2 m_j^2 - 3m_i^2 - 3m_j^2 - 1\right)$$

$$+2\beta^3\left(1-m_i^2\right)\left(1-m_j^2\right)\sum_k J_{ik}J_{kj}m_k\left(1-m_k^2\right)\left(J_{ik}m_i+J_{kj}m_j\right)+\mathcal{O}\left(J_{ij}^4\right)$$

$$+\beta^3\left(1-m_i^2\right)\left(1-m_j^2\right)\sum_{k\neq j}\sum_{l\neq i}J_{ik}J_{kl}J_{lj}\left(1-m_k^2\right)\left(1-m_l^2\right) \tag{45}$$

and

$$m_{ii}^{(B)}=1+\beta^3\left(1-m_i^2\right)^2\sum_{j\neq i}\sum_{k\neq i}J_{ij}J_{jk}J_{ki}\left(1-m_j^2\right)\left(1-m_k^2\right)+\mathcal{O}\left(J_{ij}^4\right)$$

$$=1+\mathcal{O}\left(J_{ij}^3\right). \tag{46}$$

From equation (41), one finds that ξ_{ij} only includes the contributions of neighboring pairs of nodes. In contrast, $m_{ij}^{(B)}$ includes a wider range of contributions of nodes including some loops. This is an important point when considering the approximate accuracies of both ξ_{ij} and $m_{ij}^{(B)}$. Welling and Teh compared the approximate accuracies of both approximations in their numerical experiment and concluded that the correlation function estimated by $m_{ij}^{(B)}$ is more precise than ξ_{ij} for neighboring pair of nodes [13]. Therefore, we found that a wide range of contributions of nodes play an important role in achieving approximate accuracy.

For non-neighboring pair of nodes i and j, $\xi_{ij}=m_im_j$, while

$$m_{ij}^{(B)}=m_im_j+\beta^2\left(1-m_i^2\right)\left(1-m_j^2\right)\sum_k J_{ik}J_{kj}\left(1-m_k^2\right)$$

$$+2\beta^3\left(1-m_i^2\right)\left(1-m_j^2\right)\sum_k J_{ik}J_{kj}m_k\left(1-m_k^2\right)\left(J_{ik}m_i+J_{kj}m_j\right)$$

$$+\beta^3\left(1-m_i^2\right)\left(1-m_j^2\right)\sum_{k\neq j}\sum_{l\neq i}J_{ik}J_{kl}J_{lj}\left(1-m_k^2\right)\left(1-m_l^2\right)+\mathcal{O}\left(J_{ij}^4\right). \tag{47}$$

For non-neighboring pairs of nodes, ξ_{ij} does not take the dependence between S_i and S_j into account, while $m_{ij}^{(B)}$ does. Tanaka combined the CVM and the LRR to calculate the correlation functions within the framework of the CVM, and his numerical experiments showed that his method provides good estimates of the correlation function between random variables on distant nodes [14]. The fact that $m_{ij}^{(B)}$ takes the dependence of non-neighboring pairs of nodes into account explains why Tanaka's method gives good results. Although his formulations used a more general framework of the CVM than the Bethe approximation [14], we are of the opinion that his method works well essentially because it conforms to the principles discussed in this section.

Using the framework of *the cavity method*, Montanari and Rizzo added the contributions of higher-order correlation functions to the Bethe approximation to compute loop corrections [17]. They employed the approximate LRR to estimate correlation functions, and thus the lowest-order the correlation functions called 'two-point correlation functions' in their paper correspond to $m_{ij}^{(B)}$ s. Since $m_{ij}^{(B)}$ includes the contributions of some loops, it can be expected that the contributions of the correlation functions work effectively to compute loop corrections in their method.

6. Concluding remarks

In the present paper, we showed the exact form of the correlation functions in terms of the perturbation expansion with respect to weighted links and the mathematical structure of the approximate LRR by using the naive mean-field approximation, the TAP equation and the

Bethe approximation. A comparison of the correlation functions of the exact expansions with those of the approximate LRR showed that they have similar forms in higher-order terms. This means that the approximate LRR can effectively consider effects of surrounding nodes. We found that these similarities make the approximate LRR a good approximation. Moreover, we have explained that the approximate LRR is effective when used in the CVM because the approximate LRR for the CVM can treat higher-order correlations which are not treated directly by the CVM only.

Remark that the effectiveness of the approximate LRR argued in the present paper assumes that the approximate accuracy of $\{m_i\}$ is good. For instance, the exact expanded forms of the correlation functions obtained by Plefka's expansion in equation (24) provide the exact correlation functions when $\{m_i\}$ take exact values. Thus, higher-order correlations treated by the approximate LRR should behave effectively when $\{m_i\}$ take values close to exact values. If the approximate accuracy of $\{m_i\}$ is poor, the approximate LRR cannot be guaranteed to provide a good approximation. We discussed the contributions of the higher-order terms of the first-order approximate LRR using a simple system in section 4.1. However, for more complex systems, the contributions of the higher-order terms are anticipated to be more complex and the effectiveness of terms omitted in the approximate LRR may be significant. To clarify the effectiveness of the approximate LRR for more complex systems, this will be the object of our future work.

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Appendix A. Derivation of equation (32)

In this appendix, we show the derivation of equation (32). To expand $\chi^{(1)}$ with respect to J_{ij} s, we obtain the following series:

$$\chi^{(1)} = \chi^{(1)}|_{J=\mathbf{0}} + \sum_{n=1}^{\infty} \frac{1}{n!} \sum_{(i_1 j_1)} \cdots \sum_{(i_n j_n)} \frac{\partial^n \chi^{(1)}}{\partial J_{i_1 j_1} \cdots \partial J_{i_n j_n}}\bigg|_{J=\mathbf{0}} J_{i_1 j_1} \cdots J_{i_n j_n}. \tag{A.1}$$

From equation (27), if all J_{ij}'s are equal to zero, i.e., $\boldsymbol{J} = \mathbf{0}$, we get

$$\chi^{(1)}|_{J=\mathbf{0}} = (\boldsymbol{A}^{(1)})^{-1}|_{J=\mathbf{0}} = \operatorname{diag}\left(\beta\left(1-m_1^2\right), \ldots, \beta\left(1-m_N^2\right)\right) \equiv \boldsymbol{D}^{(1)}. \tag{A.2}$$

Since the element kl of the matrix $\partial \boldsymbol{A}^{(1)}/\partial J_{ij}$ is $-\delta_{ij,kl}$ which is Kronecker's delta defined as follows

$$\delta_{ij,kl} = \begin{cases} 1 & ((ij) \text{ and } (kl) \text{ represent the same link}) \\ 0 & (\text{otherwise}), \end{cases} \tag{A.3}$$

we obtain the first-order terms of equation (A.1):

$$\sum_{(i_1 j_1)} \frac{\partial \chi^{(1)}}{\partial J_{i_1 j_1}}\bigg|_{\boldsymbol{J}=\mathbf{0}} = -\sum_{(i_1 j_1)} \chi^{(1)} \frac{\partial \boldsymbol{A}^{(1)}}{\partial J_{i_1 j_1}} \chi^{(1)}\bigg|_{\boldsymbol{J}=\mathbf{0}} = (-1) \sum_{(i_1 j_1)} \boldsymbol{D}^{(1)} \frac{\partial \boldsymbol{A}^{(1)}}{\partial J_{i_1 j_1}} \boldsymbol{D}^{(1)}. \tag{A.4}$$

The second-order terms of equation (A.1) are

$$\frac{1}{2!}\sum_{(i_1j_1)}\sum_{(i_2j_2)}\frac{\partial^2\boldsymbol{\chi}^{(1)}}{\partial J_{i_1j_2}\partial J_{i_2j_2}}\bigg|_{\boldsymbol{J}=\boldsymbol{0}}=\frac{1}{2!}\sum_{(i_1j_1)}\sum_{(i_2j_2)}\boldsymbol{D}^{(1)}\frac{\partial\boldsymbol{A}^{(1)}}{\partial J_{i_1j_1}}\boldsymbol{D}^{(1)}\frac{\partial\boldsymbol{A}^{(1)}}{\partial J_{i_2j_2}}\boldsymbol{D}^{(1)}$$
$$+\frac{1}{2!}\sum_{(i_1j_1)}\sum_{(i_2j_2)}\boldsymbol{D}^{(1)}\frac{\partial\boldsymbol{A}^{(1)}}{\partial J_{i_2j_2}}\boldsymbol{D}^{(1)}\frac{\partial\boldsymbol{A}^{(1)}}{\partial J_{i_1j_1}}\boldsymbol{D}^{(1)}$$
$$=(-1)^2\sum_{(i_1j_1)}\sum_{(i_2j_2)}\boldsymbol{D}^{(1)}\frac{\partial\boldsymbol{A}^{(1)}}{\partial J_{i_1j_1}}\boldsymbol{D}^{(1)}\frac{\partial\boldsymbol{A}^{(1)}}{\partial J_{i_2j_2}}\boldsymbol{D}^{(1)},\tag{A.5}$$

since all elements of the matrix $\partial^2\boldsymbol{A}^{(1)}/\partial J_{ij}\partial J_{kl}$ are zero. The third-order terms of equation (A.1) are

$$\frac{1}{3!}\sum_{(i_1j_1)}\sum_{(i_2j_2)}\sum_{(i_3j_3)}\frac{\partial^3\boldsymbol{\chi}^{(1)}}{\partial J_{i_1j_2}\partial J_{i_2j_2}\partial J_{i_3j_3}}\bigg|_{\boldsymbol{J}=\boldsymbol{0}}$$
$$=(-1)^3\sum_{(i_1j_1)}\sum_{(i_2j_2)}\sum_{(i_3j_3)}\boldsymbol{D}^{(1)}\frac{\partial\boldsymbol{A}^{(1)}}{\partial J_{i_1j_1}}\boldsymbol{D}^{(1)}\frac{\partial\boldsymbol{A}^{(1)}}{\partial J_{i_2j_2}}\boldsymbol{D}^{(1)}\frac{\partial\boldsymbol{A}^{(1)}}{\partial J_{i_3j_3}}\boldsymbol{D}^{(1)}.\tag{A.6}$$

All terms of the higher-order derivatives above the second-order vanish. Therefore, we obtain the nth-order terms of equation (A.1) as follows:

$$\frac{1}{n!}\sum_{(i_1j_1)}\cdots\sum_{(i_nj_n)}\frac{\partial^n\boldsymbol{\chi}^{(1)}}{\partial J_{i_1j_1}\cdots\partial J_{i_nj_n}}\bigg|_{\boldsymbol{J}=\boldsymbol{0}}$$
$$=(-1)^n\sum_{(i_1j_1)}\cdots\sum_{(i_nj_n)}\boldsymbol{D}^{(1)}\frac{\partial\boldsymbol{A}^{(1)}}{\partial J_{i_1j_1}}\boldsymbol{D}^{(1)}\frac{\partial\boldsymbol{A}^{(1)}}{\partial J_{i_2j_2}}\boldsymbol{D}^{(1)}\cdots\boldsymbol{D}^{(1)}\frac{\partial\boldsymbol{A}^{(1)}}{\partial J_{i_nj_n}}\boldsymbol{D}^{(1)}.\tag{A.7}$$

Therefore, we obtain the expanding form of the matrix $\boldsymbol{\chi}^{(1)}$ as follows:

$$\boldsymbol{\chi}^{(1)}=\boldsymbol{D}^{(1)}+\sum_{n=1}^{\infty}(-1)^n\sum_{(i_1j_1)}\cdots\sum_{(i_nj_n)}\boldsymbol{D}^{(1)}\frac{\partial\boldsymbol{A}^{(1)}}{\partial J_{i_1j_1}}\boldsymbol{D}^{(1)}\frac{\partial\boldsymbol{A}^{(1)}}{\partial J_{i_2j_2}}\boldsymbol{D}^{(1)}\cdots\boldsymbol{D}^{(1)}\frac{\partial\boldsymbol{A}^{(1)}}{\partial J_{i_nj_n}}\boldsymbol{D}^{(1)}$$
$$\times J_{i_1j_1}\cdots J_{i_nj_n}.\tag{A.8}$$

Using equation (A.8), we obtain equation (32).

Appendix B. Derivation of G_B in equation (42)

The Bethe–Helmholtz free energy is given by

$$F_B(\boldsymbol{h},\boldsymbol{J},\beta)=-\sum_i h_im_i-\sum_{(ij)}J_{ij}\xi_{ij}+\frac{1}{\beta}\sum_i(1-z_i)\sum_{S_i=\pm1}\frac{1+S_im_i}{2}\ln\frac{1+S_im_i}{2}$$
$$+\frac{1}{\beta}\sum_{(ij)}\sum_{S_i,S_j=\pm1}\frac{1+S_im_i+S_jm_j+S_iS_j\xi_{ij}}{4}\ln\frac{1+S_im_i+S_jm_j+S_iS_j\xi_{ij}}{4},\tag{B.1}$$

where m_i and ξ_{ij} are determined so as to satisfy $\partial F_B/\partial m_i=\partial F_B/\partial\xi_{ij}=0$ and z_i is defined as the number of neighbors of node i. m_i and ξ_{ij} are regarded as functions of $\boldsymbol{h}$, $\boldsymbol{J}$ and β.

Note that $\partial F_B/\partial \xi_{ij} = 0$ leads to equation (40). To apply equation (41) into F_B, we obtain

$$F_B(\boldsymbol{h}, \boldsymbol{J}, \beta) = \frac{1}{\beta} \sum_i \sum_{S_i=\pm 1} \frac{1+S_i m_i}{2} \ln \frac{1+S_i m_i}{2} - \sum_i h_i m_i - \sum_{(ij)} J_{ij} m_i m_j$$
$$- \frac{\beta}{2} \sum_{(ij)} J_{ij}^2 \left(1-m_i^2\right)\left(1-m_j^2\right) - \frac{2\beta^2}{3} \sum_{(ij)} J_{ij}^3 m_i m_j \left(1-m_i^2\right)\left(1-m_j^2\right)$$
$$- \frac{\beta^3}{12} \sum_{(ij)} J_{ij}^4 \left(1-m_i^2\right)\left(1-m_j^2\right)\left(15 m_i^2 m_j^2 - 3m_i^2 - 3m_j^2 - 1\right) + \mathcal{O}\left(J_{ij}^5\right). \quad \text{(B.2)}$$

The above calculations are discussed particularly in [16]. To obtain the Bethe–Gibbs free energy (42), we employ equation (B.2) instead of equation (B.1).

Since $\partial F_B/\partial m_i = 0$ and $\{m_i\}$ are functions of $\boldsymbol{h}$,

$$\frac{\partial F_B}{\partial h_i} = -m_i + \sum_k \frac{\partial F_B}{\partial m_k} \frac{\partial m_k}{\partial h_i} = -m_i. \quad \text{(B.3)}$$

Therefore, we obtain the Bethe–Gibbs free energy, which is the Legendre transform of the Bethe–Helmholtz free energy (B.2), as follows:

$$G_B(\boldsymbol{m}, \boldsymbol{J}, \beta) = F_B + \sum_i h_i m_i. \quad \text{(B.4)}$$

This leads to the expression of G_B in equation (42).

References

[1] Nishimori H 2001 *Statistical Physics of Spin Glass and Information Processing—An Introduction* (Oxford: Oxford University Press)
[2] Opper M and Saad D (ed) 2001 *Advanced Mean Field Methods—Theory and Practice* (Cambridge, MA: MIT Press)
[3] Plefka T 1982 *J. Phys. A: Math. Gen.* **15** 1971–8
[4] Morita T and Horiguchi T 1976 *Solid State Commun.* **19** 833–5
[5] Thouless D J, Anderson P W and Palmer R G 1977 *Phil. Mag.* **35** 593–601
[6] Ackley D H, Hinton G E and Sejowski T J 1985 *Cogn. Sci.* **9** 147–69
[7] Kappen H J and Rodríguez F B 1998 *Nueral Comput.* **10** 1137–56
[8] Leisink M A R and Kappen H J 2000 *Neural Netw.* **13** 329–35
[9] Tanaka T 1998 *Phys. Rev.* E **58** 2302–10
[10] Højen-Sørensen P A d F R, Winther O and Hansen L K 2002 *Nueral Comput.* **14** 889–918
[11] Pelizzola A 2005 *J. Phys. A: Math. Gen.* **38** R309–39
[12] Georges A and Yedidia J S 1991 *J. Phys. A: Math. Gen.* **24** 2173–92
[13] Welling M and Teh Y W 2003 *Artif. Intell.* **143** 19–50
[14] Tanaka K 2003 *IEICE Trans. Inf. Syst.* E **86-D** 1228–42
[15] Nakanishi K and Takayama H 1997 *J. Phys. A: Math. Gen.* **30** 8085–94
[16] Yasuda M and Tanaka K 2006 *J. Phys. Soc. Japan* **75** 1–8
[17] Montanari A and Rizzo T 2005 *J. Stat. Mech.* P10011