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Higher-order correlation functions of nonuniform Ising chain

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We suggest algorithms for calculating arbitrary order correlation functions $\langle S_{i_1} \dots S_{i_n} \rangle^{\mathrm{c}}$ and distribution functions $\langle S_{i_1} \dots S_{i_n} \rangle$ of a nonuniform Ising chain.

Key words: *nonuniform Ising chain, correlation functions, distribution functions*

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In this paper we consider a nonuniform Ising chain (free ends) described by the Hamiltonian

$$-\beta\,\mathcal{H} = H = \sum_{i=1}^{N} h_i S_i + \sum_{i=1}^{N-1} K_i S_i S_{i+1}\,. \tag{1}$$

Partition function of a uniform ring ($h_i = h, K_i = K$) was originally calculated by Ising [1]. General expressions for distribution functions (DFs) $\langle S_{i_1} \cdots S_{i_n} \rangle$ of an arbitrary order were suggested in [2]. Those expressions contain some unknown coefficients to be found from a cumbersome system of equations. They have been calculated only for $n = 2, 3, 4$, while for $n = 3, 4$ some of the obtained results were incorrect. However, for a nonuniform 1D model, the exact solutions exist only for a few special examples or in some limiting cases, such as zero temperature, certain disorder types, etc (see [3] and references therein). For instance, in [4] the averaged pair DFs were calculated for a binary substitution alloy at $h_i = 0$. The aim of the present paper is to formulate the diagrammatic rules for calculating arbitrary order DFs and correlation functions (CFs) $\langle S_{i_1} \cdots S_{i_n} \rangle^{\mathrm{c}}$ (cumulant average).

We shall proceed from an exact expression for generating $\mathcal{F}$-function (logarithm of partition function) of the Ising chain

$$\mathcal{F}(\{h\}) = -\sum_{i=2}^{N-1} F_i(\tilde{h}_i) + \sum_{i=1}^{N-1} F_{i,i+1}(\_\tilde{h}_i|_+\tilde{h}_{i+1}). \tag{2}$$

Here, the one-particle F_i and two-particle $F_{i,j}$ $\mathcal{F}$-functions are calculated with the one-particle H_i and two-particle $H_{i,i+1}$ Hamiltonians

$$\begin{aligned} &H_i = \tilde{h}_i S_i; \qquad \tilde{h}_i = h_i +_- \varphi_i +_+ \varphi_i\,, \\ &H_{i,i+1} = {}_-\tilde{h}_i S_i +{}_+\tilde{h}_{i+1} S_{i+1} + K_i S_i S_{i+1}\,, \\ &{}_-\tilde{h}_i = h_i +{}_-\varphi_i; \qquad {}_+\tilde{h}_{i+1} = h_{i+1} +{}_+\varphi_{i+1} \end{aligned} \tag{3}$$

and read

$$F_i(\tilde{h}_i) = F_i^{(0)} = \ln\{2\cosh\tilde{h}_i\}; \tag{4}$$

$$F_{i,i+1} = F_{i,i+1}^{(00)} = \ln\left\{2\mathrm{e}^{K_{i,i+1}}\cosh({}_-\tilde{h}_i +{}_+\tilde{h}_{i+1}) + 2\mathrm{e}^{-K_{i,i+1}}\cosh({}_-\tilde{h}_i -{}_+\tilde{h}_{i+1})]\right\}. \tag{5}$$

The fields ${}_\alpha\varphi_i$, $(\alpha = +,-)$ depend on the Hamiltonian parameters for the right-hand $(+)$ or the left-hand $(-)$ (in respect to the site i) branches of the chain and thus describe the effect of the right (left) branch of the chain on the ith spin. Obviously, ${}_-\varphi_1 =_+ \varphi_N = 0$. The rest of $2N-2$ unknown fields ${}_\alpha\varphi_i$ can be found from $2N-2$ independent relations (because of the imposed $2N$ relations $\mathrm{Sp}_{S_i}\rho_i(S_i) = \mathrm{Sp}_{S_i,S_r}\rho_{ir}(S_i,S_r)$) between the one-particle ρ_i and the two-particle $\rho_{i,r}$ density matrices

$$\rho_i(S_i) = \mathrm{Sp}_{S_r}\rho_{ir}(S_i,S_r); \quad r = i\pm 1. \tag{6}$$

Here, ρ_i and $\rho_{i,r}$ are constructed based on H_i and $H_{i,r}$, respectively. They can be written in a different form coinciding with the expressions obtained in [3]

$$\mathcal{F}(\{h\}) = \frac{1}{2}\sum_{i=1}^{N}\ln[{}_-X_i^{-1} + {}_-X_i + 2\,\cosh 2K_{i,i+1}\,], \tag{7}$$

$$\mathrm{e}^{2\,{}_-\tilde{h}_i} = {}_-X_i = [{}_-X_{i-1}\mathrm{e}^{2K_{i,i+1}} + 1]\,[{}_-X_{i-1} + \mathrm{e}^{2K_{i,i+1}}]^{-1}; \quad 2 \leqslant i \leqslant N. \tag{8}$$

Hereafter we use the following notations

$$\mathcal{F}_{i_1\ldots i_n}^{(n)}(\{h\}) = \langle S_{i_1}\ldots S_{i_n}\rangle^{\mathrm{c}} = \frac{\delta}{\delta h_{i_1}}\ldots\frac{\delta}{\delta h_{i_n}}\mathcal{F}(\{h\}), \tag{9}$$

$$F_i^{(n)} = \frac{\partial^n}{\partial(x_i)^n}F_i^{(0)}(x_i); \qquad F_{i,r}^{(nm)} = \frac{\partial^n}{\partial(x_i)^n}\frac{\partial^m}{\partial(y_r)^m}F_{i,r}^{(00)}(x_i \mid y_r). \tag{10}$$

The following form of the system (6) will be used

$$\mathcal{F}_i^{(1)}(\{h\}) = F_i^{(1)}(\tilde{h}_i) = F_{i,i\pm1}^{(10)}({}_\mp\tilde{h}_i|_\pm\tilde{h}_{i\pm1}). \tag{11}$$

Relations (11) can be also obtained proceeding from the stationarity condition for $\mathcal{F}(\{h\})$ with respect to ${}_\alpha\varphi_1$ $(\frac{\partial}{\partial_\alpha\varphi_i}\mathcal{F}(\{h\}) = 0)$. In the case of an infinite chain and a uniform field $(h_i = h,\ {}_-\varphi_i =\ {}_+\varphi_{i+1} = \varphi)$ the thermodynamic quantities in (7), (8) and (11) are independent of the site index i. Solving the equation (8) with respect

to $_{-}\tilde{h}$ and substituting the obtained expression into (7) and (11), we get the known formulas

$$\frac{\mathcal{F}}{N} = K + \ln[\cosh K + r], \tag{12}$$

$$\langle S_i \rangle = \frac{\sinh(h)}{r}; \qquad r = \sqrt{\mathrm{e}^{-2K} + \sinh^2(h)}. \tag{13}$$

Hereafter we consider only the right-hand (in respect to the site i) branch of a chain. Differentiating (11) with respect to h_{i+n}, $(n \geqslant 0)$ and taking into account the fact that $\frac{\delta}{\delta h_{i+n}}\ {}_{-}\tilde{h}_i = \delta_{i,i+n}$, we obtain an equation for $\frac{\delta}{\delta h_{i+n}}\ {}_{+}\tilde{h}_i = \frac{\delta}{\delta h_{i+n}}\ \tilde{h}_i$. It can be solved by iterating procedure and permits to find the expression for the pair CF

$$\mathcal{F}^{(2)}_{i,i+n} = \frac{\delta}{\delta h_{i+n}} F^{(1)}_i = F^{(2)}_i \frac{\delta}{\delta h_{i+n}} \tilde{h}_i = F^{(2)}_i f_{i,i+1} \cdots f_{i+n-1,i+n} \overset{h_i = h}{\Rightarrow} F^{(2)}\, f^n, \tag{14}$$

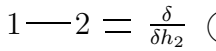
where

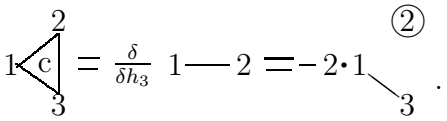
$$f_{i,i+1} = \frac{F^{(11)}_{i,i+1}}{F^{(20)}_{i,i+1}} \overset{h_i = h}{\Rightarrow} f = [\cosh(h) - r]\,[\cosh(h) + r]^{-1}. \tag{15}$$

The expression for ternary CF is derived by differentiating (14)

$$\mathcal{F}^{(3)}_{i,i+n,i+k} = \frac{\delta}{\delta h_{i+k}} \mathcal{F}^{(2)}_{i,i+n} = -2\mathcal{F}^{(1)}_{i+n} \mathcal{F}^{(2)}_{i,i+k} \overset{h_i = h}{\Rightarrow} F^{(3)}\, f^k\,. \tag{16}$$

As follows from relations (14) and (16), the higher CFs invoke only the single-particle $\mathcal{F}^{(1)}_i$ and the pair $\mathcal{F}^{(2)}_{i,j}$ CFs. It is convenient to present these relations in a diagram form (below we use the notations $i_1 = 1 \leqslant i_2 = 2 \leqslant i_3 = 3 \leqslant \cdots$)

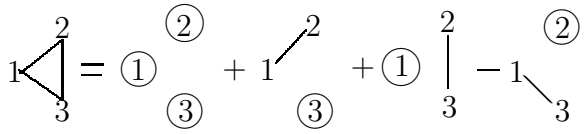
$\mathcal{F}^{(2)}_{1,2} = \frac{\delta}{\delta h_2} \mathcal{F}^{(1)}_1 \quad \Longleftrightarrow$ 

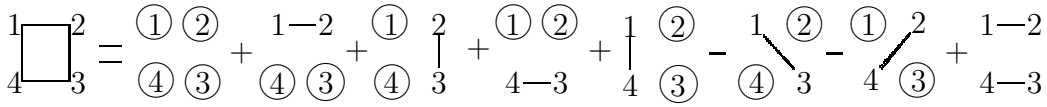
$\mathcal{F}^{(3)}_{1,2,3} = \frac{\delta}{\delta h_3} \mathcal{F}^{(2)}_{1,2} = -2\mathcal{F}^{(1)}_2 \mathcal{F}^{(2)}_{1,3} \quad \Longleftrightarrow$ 

First, we find the higher DFs from the recurrent relation

$$\langle S_1 \cdots S_n S_{n+1} \rangle = \frac{\delta}{\delta h_{n+1}} \langle S_1 \cdots S_n \rangle + \langle S_1 \cdots S_n \rangle \langle S_{n+1} \rangle. \tag{17}$$

Thus, we obtain expressions for $\langle S_1 S_2 S_3 \rangle$ and $\langle S_1 S_2 S_3 S_4 \rangle$





In a uniform case, these diagrams are rewritten as follows:

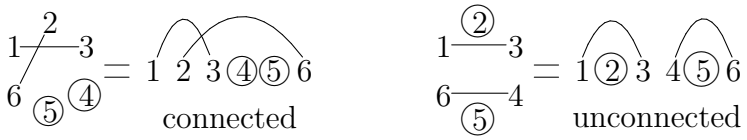
$$\langle S_1 S_2 S_3 \rangle = [F^{(1)}]^3 + F^{(1)} F^{(2)} [f^{2-1} + f^{3-2} - f^{3-1}], \tag{18}$$

$$\langle S_1 S_2 S_3 S_4 \rangle = [F^{(1)}]^4 + [F^{(1)}]^2 F^{(2)} [f^{2-1} + f^{3-2} + f^{4-3} + f^{4-1} - f^{3-1} - f^{4-2}] + [F^{(2)}]^2 f^{2-1} f^{4-3}. \tag{19}$$

In the particular case of the nearest neighbors, the DFs (18) and (19) coincide with those obtained in [5]. The same formulae can be also derived by using the transfer matrix method. In contrast to the present results, all the terms in the expressions for $\langle S_1 S_2 S_3 \rangle$ and $\langle S_1 S_2 S_3 S_4 \rangle$ obtained in [2] occur only with the plus signs and are incorrect, as we have already mentioned earlier.

Starting from (17) and using the mathematic induction method, we can formulate general rules for calculating the DFs of an arbitrary order. The DFs $\langle S_1 S_2 \cdots S_n \rangle$ are the sums of all diagrams with n vertices, obeying the following conditions.

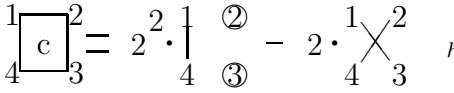
- A diagram should consist of free vertices (i) $= \langle S_i \rangle$ and bonds i−j $= \langle S_i S_j \rangle^{\mathrm{c}}$.
- A diagram is unconnected along the line $1, 2, \cdots, \mathsf{n}$.



- Each bond i−j gives the coefficient $(-1)^{j-i-1}$ where $(j-i-1)$ is the number of vertices between the sites i and j.

Similar rules can be also derived by using the transfer matrix method.

The higher CFs are obtained from (9), (14) and (16). For instance, $\langle S_1 S_2 S_3 S_4 \rangle^{\mathrm{c}}$ reads



$$\overset{h_i=h}{\Rightarrow} \quad \langle S_1 S_2 S_3 S_4 \rangle^{\mathrm{c}} = 2^2 [F^{(1)}]^2 F^{(2)} f^{4-1} - 2 [F^{(2)}]^2 f^{3-1} f^{4-2}.$$

As one can see, the CF, unlike the DEF, contains only the diagrams connected along the line $1, 2, \cdots, \mathsf{n}$. A thorough diagrammatic analysis of the CFs permitted to formulate the following general rules. The CF $\langle S_1 S_2 \cdots S_n \rangle^{\mathrm{c}}$ is a sum of all diagrams with n vertices, obeying the following conditions.

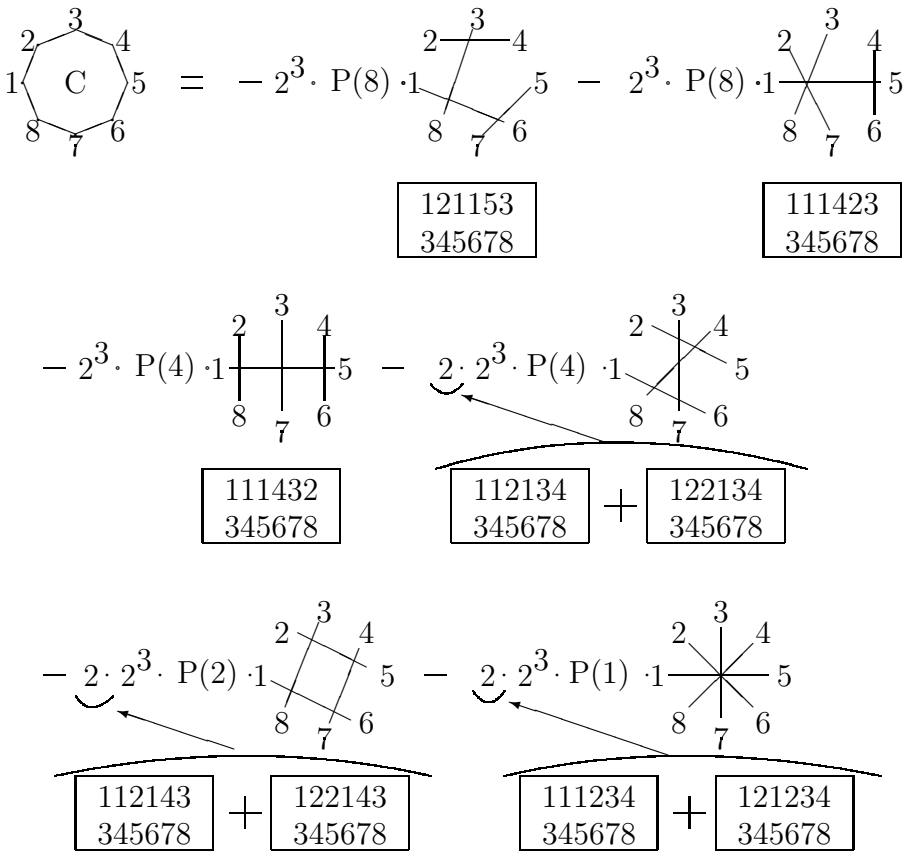
- A diagram should consist of free vertices (i) $= \langle S_i \rangle$ and bonds i−j $= \langle S_i S_j \rangle^{\mathrm{c}}$.
- A diagram should be connected along the line $1, 2, \cdots, \mathsf{n}$.

- There is always a bond $1-n$. The bonds i—$(i+1)$ for the neighbouring vertices are absent.

- A prefactor at each diagram is $(-2)^{(n-l-1)}$ where l is the number of bonds in diagram.

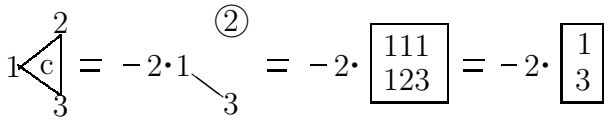
- There is an additional coefficient, arising at the differentiation and defined by a special rule.

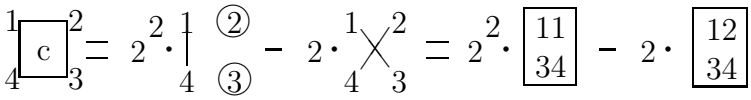
For instance, the expression for $\langle S_1 \cdots S_8 \rangle^{\mathrm{c}}$ (for simplicity at $h_i = 0$) reads



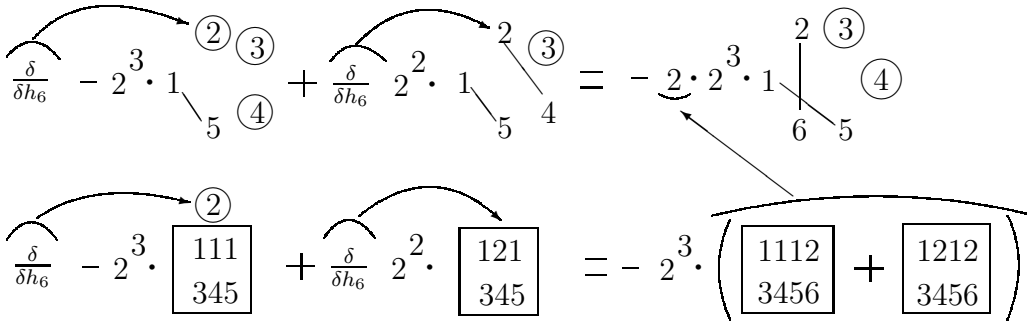
Here, the notation $P(n)$ at the diagrams stands for a sum of all nonequivalent diagrams with the same symmetry of lines. The boxes contain digital notations of the diagrams. The index i in the upper row corresponds to one of the vertices $\textcircled{i} = \langle S_i \rangle$ or bonds $i-j = \langle S_i S_j \rangle^{\mathrm{c}}$ which are differentiated with respect to h_k given by the index k in the lower row. Thus, the digital diagram reflects the differentiation procedure. For example, the expressions for $\langle S_1 S_2 S_3 \rangle^{\mathrm{c}}$ and $\langle S_1 S_2 S_3 S_4 \rangle^{\mathrm{c}}$ in digital

notations are as follows:





At a certain step of differentiation, the derivatives of different diagrams can be identical. Consider, for example, the origin of the last diagram in $\langle S_1 \cdots S_8 \rangle^{\mathrm{c}}$. The two different diagrams from $\langle S_1 \cdots S_5 \rangle^{\mathrm{c}}$ at the differentiation with respect to h_6 yield



Here, an additional coefficient **2** emerged due to the differentiation. At the differentiation of the vertices $\langle S_3 \rangle$ and $\langle S_4 \rangle$ in the present diagram with respect to h_7 and h_8, correspondingly, we obtain the last diagram in $\langle S_1 \cdots S_8 \rangle^{\mathrm{c}}$.

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Кореляційні функції Ізінгового ланцюжка вищих порядків

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Запропоновано алгоритми розрахунку кореляційний функцій ($\langle S_{i_1} \dots S_{i_n} \rangle^{\mathrm{c}}$) та функцій розподілу ($\langle S_{i_1} \dots S_{i_n} \rangle$) довільного порядку для неоднорідного Ізінгового ланцюжка.

Ключові слова: *неоднорідний Ізінговий ланцюжок, кореляційні функції, функції розподілу*

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