Moments of general Heisenberg Hamiltonians up to sixth order

Heinz-Jürgen Schmidt\textsuperscript{1}, Andre Lohmann\textsuperscript{2} and Johannes Richter\textsuperscript{2}

\textsuperscript{1} Universität Osnabrück, Fachbereich Physik, Barbarastr. 7, D - 49069 Osnabrück, Germany
\textsuperscript{2} Institut für Theoretische Physik, Otto-von-Guericke-Universität Magdeburg, PF 4120, D - 39016 Magdeburg, Germany

\textsuperscript{§} Correspondence should be addressed to hschmidt@uos.de
Abstract. We explicitly calculate the moments $t_n$ of general Heisenberg Hamiltonians up to sixth order. They have the form of finite sums of products of two factors, the first factor being represented by a multigraph and the second factor being a polynomial in the variable $s(s + 1)$, where $s$ denotes the individual spin quantum number. As an application we determine the corresponding coefficients of the expansion of the free energy and the zero field susceptibility in powers of the inverse temperature. These coefficients can be written in a form which makes explicit their extensive character.

1. Introduction

The moments of the general Heisenberg Hamiltonian describing a large class of spin systems represent valuable information for various purposes. They can be used to check numerical exact or approximate calculations of the energy spectrum of such systems. Further they directly appear in the high temperature expansion (HTE) of the partition function. Hence they can be used to calculate the leading terms of the HTE of physical relevant functions such as specific heat or magnetic susceptibility, see e. g. [1] or [2]. Analytic expression for the moments in the general Heisenberg case (arbitrary number of spins $N$ and coupling constants $J_{\mu\nu}$, arbitrary spin quantum number $s$) are interesting since they can be used to investigate the dependence of physical properties on the coupling constants even in cases where a numerical investigation is not possible due to large $N$ or $s$. It seems that such analytical expressions for moments have only be published up to order three, see [3], although the polynomials which appear in such expressions are known up to 8th order, see [1]. Those papers which consider higher order expansions are usually confined to special coupling geometries or and/or $s = 1/2$, see e. g. [4]-[17].

In this article we only give the analytical results for the moments $t_4$, $t_5$, $t_6$ without explaining the method by which we obtained them. This will be done in another paper. From these results we have determined the coefficients of the susceptibility’s HTE $c_4$, $c_5$, $c_6$ by a method which is briefly sketched. Similarly, the coefficients $a_n$ of the free energy’s series expansion (or, more precisely, of $-\beta F(\beta)$) are calculated up to 6th order in $\beta$. We have checked our results by comparison with numerical results for spin systems with random coupling coefficients and $N \leq 7$ and $s = 1/2, 1$. Moreover, our expression for $c_4$ has been checked by comparison with the published results for chains [18] and $J_1 - J_2$ square lattices [19, 20].
2. Definitions

We consider the following notations:

- \( N \) \( \quad \) Number of spins
- \( S_N \) \( \quad \) Group of permutations \( \pi : \{1, 2, \ldots, N\} \to \{1, 2, \ldots, N\} \)
- \( s = \frac{1}{2}, 1, \frac{3}{2}, \ldots \) \( \quad \) Single spin quantum number
- \( r \equiv s(s+1) \) \( \quad \) Abbreviation
- \( J_{\mu\nu} = J_{\nu\mu}, 1 \leq \mu \neq \nu \leq N \) \( \quad \) Coupling constants
- \( s_\mu \) \( \quad \) Spin vector operator of the \( \mu \)th spin
- \( S = \sum_\mu s_\mu \) \( \quad \) Total spin vector
- \( S^{(i)}, i = 1, 2, 3 \) \( \quad \) \( i \)th component of the total spin vector
- \( H = \sum_{\mu<\nu} J_{\mu\nu} s_\mu \cdot s_\nu \) \( \quad \) Heisenberg Hamilton operator
- \( (2s+1)^N \) \( \quad \) Dimension of the Hilbert space
- \( t_n = \frac{\text{Tr}(H^n)}{(2s+1)^N} \) \( \quad \) Normalized moments of \( H \)
- \( \mu_n = \frac{\text{Tr}(S^{(i)2}H^n)}{(2s+1)^N} \) \( \quad \) Normalized magnetic moments of \( H \)
- \( \beta = \frac{1}{kT} \) \( \quad \) Inverse temperature
- \( \chi(\beta) = \beta \frac{\text{Tr}(S^{(i)2}\exp(-\beta H))}{\text{Tr}(\exp(-\beta H))} \) \( \quad \) Zero field susceptibility
- \( \chi(\beta) = \sum_{n=1}^{\infty} c_n \beta^n \) \( \quad \) High temperature expansion of \( \chi(\beta) \)
- \( -\beta F(\beta) = \ln \left( \text{Tr} e^{-\beta H} \right) \) \( \quad \) Free energy \( F(\beta) \)
- \( -\beta F(\beta) = \sum_{n=0}^{\infty} a_n \beta^n \) \( \quad \) High temperature expansion of \( F(\beta) \)

In order to write our results in a compact way we will utilize some graph theoretic notations. This is a common practice when dealing with series expansions, see e. g. [2]. Let \( \mathcal{G} \) be a multigraph consisting of \( g \) nodes (vertices) and \( \mathcal{N}(i,j) = \mathcal{N}(j,i) \) bonds (edges) between the \( i \)th and the \( j \)th node. We do not consider “loops”, i. e. \( \mathcal{N}(i,i) = 0 \) for all \( i = 1, \ldots, g \). The total number of all bonds, \( \gamma(\mathcal{G}) = \sum_{i<j} \mathcal{N}(i,j) \) will be called the size of \( \mathcal{G} \). \( \mathcal{G} \) is not necessarily connected, see the examples of multigraphs below. We will identify the set of \( g \) nodes with \( \{1, 2, \ldots, g\} \) and the set of \( N \) spins with \( \{1, 2, \ldots, N\} \).

All multigraphs \( \mathcal{G}_\nu, \nu = 1, \ldots, 86 \) needed in this paper are represented in table I.

From the expansion

\[
\text{Tr} \ H^n = \sum_{\mu_1<\nu_1, \ldots, \mu_n<\nu_n} \prod_i J_{\mu_i\nu_i} \text{Tr} \left( \prod_i s_{\mu_i} \cdot s_{\nu_i} \right) \quad (1)
\]

it is clear that the expressions for the moments \( t_n \) involve various products of coupling constants \( J_{\mu\nu} \). The structure of these products can be represented by the multigraphs \( \mathcal{G} \) defined above, such that the factors \( J^\ell_{\mu\nu} \) correspond to the bonds of \( \mathcal{G} \) with multiplicity \( \ell \). The sum of different products in (1) of the same structure will be obtained by an evaluation of \( \mathcal{G} \), denoted by \( \mathcal{G} \), for the spin system under consideration. \( \mathcal{G} \) denotes a real number which depends on the coupling constants and only implicitly on the number \( N \).
### Table 1. Multigraphs $G_\nu$

| $\nu$ | $G_\nu$ | \(\ldots\) | \(\ldots\) | \(\ldots\) | \(\ldots\) | \(\ldots\) |
|-------|---------|-------------|-------------|-------------|-------------|-------------|
| 1     |         | 9           | 17          | 25          |             |             |
| 2     |         | 10          | 18          | 26          |             |             |
| 3     |         | 11          | 19          | 27          |             |             |
| 4     |         | 12          | 20          | 28          |             |             |
| 5     |         | 13          | 21          | 29          |             |             |
| 6     |         | 14          | 22          | 30          |             |             |
| 7     |         | 15          | 23          | 31          |             |             |
| 8     |         | 16          | 24          | 32          |             |             |
| $\nu$ | $\mathcal{G}_\nu$ | ... | ... | ... | ... |
|-------|-------------------|-----|-----|-----|-----|
| 33    | ![Diagram](image1) | 41  | 49  | 57  |     |
| 34    | ![Diagram](image2) | 42  | 50  | 58  |     |
| 35    | ![Diagram](image3) | 43  | 51  | 59  |     |
| 36    | ![Diagram](image4) | 44  | 52  | 60  |     |
| 37    | ![Diagram](image5) | 45  | 53  | 61  |     |
| 38    | ![Diagram](image6) | 46  | 54  | 62  |     |
| 39    | ![Diagram](image7) | 47  | 55  | 63  |     |
| 40    | ![Diagram](image8) | 48  | 56  | 64  |     |
| $\nu$ | $g_\nu$ | ... | ... | ... | ... | ... |
|-------|---------|-----|-----|-----|-----|-----|
| 65    |         | 71  |     | 77  |     | 83  |
| 66    |         | 72  |     | 78  |     | 84  |
| 67    |         | 73  |     | 79  |     | 85  |
| 68    |         | 74  |     | 80  |     | 86  |
| 69    |         | 75  |     | 81  |     |     |
| 70    |         | 76  |     | 82  |     |     |
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of spins. This number will be defined according to the following statements.

(i) If \( g > N \) we set \( \mathcal{G} = 0 \).

(ii) If \( g \leq N \) we consider the symmetry group \( G \) of \( \mathcal{G} \), defined by

\[
G = \{ \pi \in S_N | \pi \text{ maps } \{1, 2, \ldots, g\} \text{ onto } \{1, 2, \ldots, g\} \text{ and } \}
\]

\[
\mathcal{N}(i, j) = \mathcal{N}(\pi(i), \pi(j)) \text{ for all } 1 \leq i, j \leq g \}
\]

Further we consider the quotient set \( S_N / G \) consisting of left cosets \( \pi G, \pi \in S_N \) and choose a representative \( \pi_\ell \) from each coset, \( \pi_\ell \in \pi G, \ell = 1, \ldots, L \equiv |S_N / G| = \frac{N!}{|G|} \).

(iii) Then we define

\[
\mathcal{G} \equiv \sum_{\ell=1}^{L} \prod_{1 \leq i < j \leq g} (J_{\pi_\ell(i), \pi_\ell(j)})^{\mathcal{N}(i, j)}.
\]

Obviously, the definition of \( \mathcal{G} \) does not depend on the choice of representatives \( \pi_\ell \) since the product \( \prod_{1 \leq i < j \leq g} (J_{\pi_\ell(i), \pi_\ell(j)})^{\mathcal{N}(i, j)} \) is invariant under permutations from the symmetry group \( \pi \in G \).

In order to illustrate this definition we consider an example of \( N = 4 \) spins and

\[
G = \Delta, \text{ hence } g = 3 < 4 = N. \text{ The symmetry group } G \text{ consists of all permutations of } \{1, 2, 3, 4\} \text{ leaving } 4 \text{ fixed, hence } |G| = 3! = 6. \text{ Thus we have } L = \frac{4!}{3!} = 4 \text{ left cosets from which we choose the representatives } \pi_1 = (1)(2)(3)(4) = id, \pi_2 = (1234), \pi_3 = (13)(24), \pi_4 = (1432). \text{ Hence } \mathcal{G} = J_{12}J_{23}J_{13} + J_{23}J_{34}J_{23} + J_{34}J_{14}J_{13} + J_{14}J_{12}J_{24}.
\]

The coefficients \( c_n \) of the susceptibility’s HTE (and similarly the \( a_n \) of the free energy HTE) will contain products of evaluations \( \mathcal{G}_\nu, \mathcal{G}_\mu \). These expressions can be simplified using rules which transform such products into linear combinations of other evaluations. To give an example, we consider

\[
\mathcal{G}_1 \mathcal{G}_2 = \mathcal{G}_4 + \mathcal{G}_5 + \mathcal{G}_6,
\]

\[
\mathcal{G}_2^2 = \mathcal{G}_9 + 2\mathcal{G}_{12} + 2\mathcal{G}_{17},
\]

\[
\mathcal{G}_2 \mathcal{G}_3 = \mathcal{G}_{10} + \mathcal{G}_{13} + \mathcal{G}_{14} + \mathcal{G}_{16} + \mathcal{G}_{18},
\]

\[
\mathcal{G}_3 \mathcal{G}_4 = \mathcal{G}_9 + \mathcal{G}_{10} + \mathcal{G}_{11},
\]

\[
\mathcal{G}_2 \mathcal{G}_4 = \mathcal{G}_{23} + \mathcal{G}_{26} + \mathcal{G}_{31},
\]

Similar expressions can be derived for other products of evaluations where suitable coefficients will compensate the change of symmetry groups. For the purpose of the present paper we will need the following “product rules”:

\[
\mathcal{G}_1 \mathcal{G}_2 = \mathcal{G}_4 + \mathcal{G}_5 + \mathcal{G}_6,
\]

\[
\mathcal{G}_2^2 = \mathcal{G}_9 + 2\mathcal{G}_{12} + 2\mathcal{G}_{17},
\]

\[
\mathcal{G}_2 \mathcal{G}_3 = \mathcal{G}_{10} + \mathcal{G}_{13} + \mathcal{G}_{14} + \mathcal{G}_{16} + \mathcal{G}_{18},
\]

\[
\mathcal{G}_3 \mathcal{G}_4 = \mathcal{G}_9 + \mathcal{G}_{10} + \mathcal{G}_{11},
\]

\[
\mathcal{G}_2 \mathcal{G}_4 = \mathcal{G}_{23} + \mathcal{G}_{26} + \mathcal{G}_{31},
\]
\[ G_1 G_7 = \overline{G}_{14} + \overline{G}_{19} + \overline{G}_{20}, \]  
\[ G_2 G_4 = \overline{G}_{23} + \overline{G}_{26} + \overline{G}_{31}, \]  
\[ G_3 G_4 = \overline{G}_{24} + \overline{G}_{27} + \overline{G}_{28} + \overline{G}_{30} + \overline{G}_{32}, \]  
\[ G_4^2 = \overline{G}_{58} + 2\overline{G}_{62} + 2\overline{G}_{66}, \]  
\[ G_2 G_5 = \overline{G}_{24} + \overline{G}_{26} + 2\overline{G}_{33} + 2\overline{G}_{34} + \overline{G}_{35} + 2\overline{G}_{44} + \overline{G}_{46}, \]  
\[ G_2 G_6 = \overline{G}_{25} + \overline{G}_{31} + 2\overline{G}_{35} + 2\overline{G}_{36} + \overline{G}_{46} + 2\overline{G}_{47}, \]  
\[ G_3 G_7 = \overline{G}_{28} + \overline{G}_{38} + \overline{G}_{48}, \]  
\[ G_2 G_8 = \overline{G}_{34} + \overline{G}_{37} + \overline{G}_{50} + 2\overline{G}_{51} + \overline{G}_{52} + \overline{G}_{54}, \]  
\[ G_2 G_7 = \overline{G}_{60} + \overline{G}_{64} + 2\overline{G}_{67}, \]  
\[ G_7^2 = \overline{G}_{70} + 2\overline{G}_{74} + 2\overline{G}_{83} + 2\overline{G}_{85}, \]  
\[ G_2 G_8 = \overline{G}_{49} + \overline{G}_{29} + \overline{G}_{30} + \overline{G}_{37} + \overline{G}_{39} + \overline{G}_{42} + \overline{G}_{45}, \]  
\[ G_1 G_9 = \overline{G}_{23} + \overline{G}_{24} + \overline{G}_{25}, \]  
\[ G_3 G_9 = \overline{G}_{58} + \overline{G}_{59} + \overline{G}_{61}, \]  
\[ G_2 G_{12} = \overline{G}_{59} + 3\overline{G}_{68} + 3\overline{G}_{70} + 2\overline{G}_{71} + \overline{G}_{73}, \]  
\[ G_7 G_{12} = \overline{G}_{26} + \overline{G}_{33} + \overline{G}_{34} + \overline{G}_{35} + \overline{G}_{36}, \]  
\[ G_1 G_{14} = \overline{G}_{28} + 2\overline{G}_{34} + \overline{G}_{37} + \overline{G}_{40} + \overline{G}_{41}, \]  
\[ G_2 G_{14} = \overline{G}_{60} + \overline{G}_{63} + \overline{G}_{69} + \overline{G}_{76} + \overline{G}_{78}, \]  
\[ G_1 G_{17} = \overline{G}_{31} + \overline{G}_{44} + \overline{G}_{46} + \overline{G}_{47}, \]  
\[ G_2 G_{17} = \overline{G}_{61} + \overline{G}_{71} + 2\overline{G}_{73} + 3\overline{G}_{81}, \]  
\[ G_1 G_{21} = \overline{G}_{42} + 2\overline{G}_{51} + 2\overline{G}_{53} + \overline{G}_{55}, \]  
\[ G_2 G_{21} = \overline{G}_{65} + 2\overline{G}_{74} + \overline{G}_{77} + \overline{G}_{82}. \]

From these equations one can derive further ones for multiple products, for example:

\[ G_1 G_2^2 = G_{23} + G_{24} + 2\left( G_{26} + G_{33} + G_{34} + G_{35} + G_{36} + G_{31} + G_{44} + G_{47} \right). \]

3. Results

3.1. Moments

It turns out that the moments \( t_n \) can be written in the following way:

\[ t_n = \sum_{\nu \in T_n} \overline{G}_\nu p_\nu(r). \]

Here the \( G_\nu, \nu \in T_n \), denote certain multigraphs of size \( n \) and the \( p_\nu \) are polynomials of order \( \leq n \) in the variable \( r = s(s + 1) \). It is crucial that these polynomials depend neither on \( N \) nor on the coupling constants \( J_{\mu \nu} \) whereas the terms \( \overline{G}_\nu \) depend only on the coupling constants and only implicitly on \( N \) via (3). For the determination of \( t_n \) it thus
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suffices to enumerate the multigraphs $G_\nu$, $\nu \in T_n$ and the corresponding polynomials $p_\nu$. The first moments are well-known:

$$t_1 = 0$$

$$t_2 = \sum_{\mu < \nu} J_{\mu \nu}^2 \frac{1}{3} r^2 = \frac{1}{3} r^2 = G_{\bar{2}} \frac{1}{3} r^2$$

(32)

(33)

The third moment $t_3$ has been calculated in [3]. We reproduce this result using our notation and the multigraphs represented in table 1.

$$t_3 = -\frac{1}{6} r^2 G_{\bar{4}} + 2 \frac{1}{3} r^3 G_{\bar{7}}$$

(34)

The next moments $t_4$, $t_5$, $t_6$ have, to our best knowledge, not yet been published, although the polynomials which appear in these expressions are known up to 8th order, see [1].

They are given by the following expressions:

$$t_4 = \frac{1}{15} r^2(2 + r(-2 + 3r)) G_{\bar{9}} + 2 \frac{9}{9} r^3(-1 + 3r) G_{\bar{12}} - 2 \frac{9}{9} r^3 G_{\bar{14}}$$

$$+ \frac{2}{3} r^4 G_{\bar{17}} + \frac{8}{9} r^4 G_{\bar{21}},$$

(35)

$$t_5 = -\frac{1}{6} r^2(1 + 2(-1 + r)r) G_{\bar{23}} + \frac{5}{18} r^3(1 - 2r) G_{\bar{26}}$$

$$+ \frac{9}{9} r^3(3 - 8r + 12r^2) G_{\bar{28}} - \frac{9}{9} r^4 G_{\bar{31}} + \frac{20}{27} r^4(-1 + 3r) G_{\bar{38}}$$

$$- \frac{10}{27} r^4 G_{\bar{42}} + \frac{20}{9} r^5 G_{\bar{48}} + \frac{40}{27} r^5 G_{\bar{56}},$$

(36)

and

$$t_6 = \frac{1}{105} r^2(32 - 87r + 88r^2 - 30r^3 + 15r^4) G_{\bar{60}} + \frac{1}{6} r^3(-3 + 8r - 8r^2 + 6r^3) G_{\bar{59}}$$

$$- \frac{2}{3} r^3(1 - 3r + 3r^2) G_{\bar{60}} + \frac{1}{3} r^4(2 - 2r + 3r^2) G_{\bar{61}} + \frac{2}{9} r^3(-2 + 3r) G_{\bar{62}}$$

$$+ \frac{1}{3} r^4(1 - 2r) G_{\bar{63}} + \frac{10}{9} r^4(1 - 2r) G_{\bar{64}} + \frac{2}{9} r^4(3 - 8r + 12r^2) G_{\bar{65}}$$

$$+ \frac{5}{9} r^4 G_{\bar{66}} - \frac{20}{9} r^5 G_{\bar{67}} + \frac{10}{9} r^4(1 - 3r + 3r^2) G_{\bar{68}}$$

$$+ \frac{5}{9} r^4(1 - 2r) G_{\bar{69}} + \frac{1}{5} r^3(-1 + 9r - 22r^2 + 22r^3) G_{\bar{70}}$$

$$+ \frac{2}{9} r^4(2 - 10r + 15r^2) G_{\bar{71}} + \frac{2}{9} r^4 G_{\bar{72}} + \frac{10}{9} r^5 G_{\bar{73}}$$

$$+ \frac{2}{9} r^4(5 - 24r + 36r^2) G_{\bar{74}} - \frac{2}{9} r^4 G_{\bar{75}} + \frac{2}{9} r^4(1 - 5r) G_{\bar{76}}$$

$$+ \frac{40}{27} r^5(-1 + 3r) G_{\bar{77}} - \frac{10}{9} r^5 G_{\bar{78}} + \frac{1}{3} r^4 G_{\bar{79}} - \frac{20}{27} r^5 G_{\bar{80}}$$
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\[ + \frac{10}{3} r^6 \bar{G}_{81} + \frac{40}{9} r^6 \bar{G}_{82} + \frac{80}{27} r^5 (-1 + 3r) \bar{G}_{83} \\
+ \frac{2}{9} r^4 \bar{G}_{84} + \frac{80}{9} r^6 \bar{G}_{85} + \frac{80}{27} r^6 \bar{G}_{86}. \]  

(37)

3.2. Free energy

It is well-known that the coefficients of the power series for the free energy \( F(\beta) \)

\[- \beta F(\beta) = \ln (\Tr e^{-\beta H}) = \sum_{n=0}^{\infty} a_n \beta^n \]  

(38)

can be expressed in terms of the moments \( t_n \) and its products. As indicated in section 2, a variety of product rules can be used to simplify the resulting expressions. This simplification, which is sometimes also referred to as the "cumulant expansion", see [2], has the further advantage that it reveals the extensive character of the \( a_n \), see section 3.3 for a more detailed discussion. The first seven coefficients of the series (38) read as follows.

\[ a_0 = N \ln(2s + 1), \]  

(39)

\[ a_1 = 0, \]  

(40)

\[ a_2 = \frac{1}{6} r^2 \bar{G}_2, \]  

(41)

\[ a_3 = \frac{1}{36} r^2 \bar{G}_4 - \frac{1}{9} r^3 \bar{G}_7, \]  

(42)

\[ a_4 = -\frac{1}{180} r^2 (-1 + r + r^2) \bar{G}_9 - \frac{1}{108} r^3 \bar{G}_{12} - \frac{1}{108} r^3 \bar{G}_{14} + \frac{1}{27} r^4 \bar{G}_{21}, \]  

(43)

\[ a_5 = -\frac{1}{2160} r^2 (-3 + 6r + 4r^2) \bar{G}_{23} - \frac{1}{432} r^3 \bar{G}_{26} \]
\[ + \frac{1}{1080} r^3 (-3 + 8r + 8r^2) \bar{G}_{28} \]
\[ + \frac{1}{162} r^4 \bar{G}_{38} + \frac{1}{324} r^4 \bar{G}_{42} - \frac{1}{81} r^5 \bar{G}_{56}, \]  

(44)

\[ a_6 = \frac{1}{453600} r^2 (192 - 522r - 67r^2 + 240r^3 + 160r^4) \bar{G}_{58} \]
\[ + \frac{1}{12960} r^3 (-9 + 12r + 8r^2) \bar{G}_{59} + \frac{1}{1080} r^3 (-1 + 3r + 2r^2) \bar{G}_{60} \]
\[ + \frac{1}{6480} r^3 (-4 + r) \bar{G}_{62} + \frac{1}{648} r^4 (3 + 4r) \bar{G}_{63} + \frac{1}{648} r^4 \bar{G}_{64} \]
\[ - \frac{1}{3240} r^4 (-3 + 8r + 8r^2) \bar{G}_{65} + \frac{1}{648} r^4 \bar{G}_{68} \]
\[ + \frac{1}{1296} r^4 \bar{G}_{69} - \frac{1}{32400} r^3 (9 - 81r + 48r^2 + 152r^3) \bar{G}_{70} \]
\[ + \frac{1}{1620} r^4 \bar{G}_{71} + \frac{1}{3240} r^4 \bar{G}_{72} \]
\[ - \frac{1}{3240} r^4 (-5 + 24r + 24r^2) \bar{G}_{74} - \frac{1}{3240} r^4 \bar{G}_{75} \]
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\[ + \frac{1}{3240} r_4 G_{76} - \frac{1}{486} r_5 G_{77} + \frac{1}{2160} r_4 G_{79} - \frac{1}{927} r_5 G_{80} \]
\[ - \frac{1}{243} r_5 G_{83} + \frac{1}{3240} r_4 G_{84} + \frac{1}{243} r_6 G_{86}. \]  

(45)

3.3. Magnetic moments and susceptibility

To obtain the magnetic moments \( \mu_n \) we can use a special method which is available if one knows the moments \( t_n \) for all values of the coupling constants \( J_{\mu \nu} \). We replace \( H \) by the one parameter family of Hamiltonians \( H_\alpha \equiv H + \frac{\alpha}{2} (S^2 - Nr) \). Equivalently we can substitute \( J_{\mu \nu} \rightarrow J_{\mu \nu} + \alpha \) for all coupling constants. The magnetic moments then result from differentiating \( \text{Tr}(H_\alpha^n) \) w. r. t. \( \alpha \) and finally setting \( \alpha = 0 \):

\[
\frac{\partial}{\partial \alpha} \text{Tr} \left( H_\alpha^{n+1} \right) \bigg|_{\alpha=0} = \frac{n+1}{2} \text{Tr} \left( H_0^n (S^2 - Nr) \right) 
\]

(46)

\[
= \frac{(n+1)(2s+1)^N}{2} (3\mu_n - Nrt_n).
\]

(47)

We can calculate the left hand side of (46) if we insert the results for the moments and consider “derivatives” \( G' \) of multigraphs defined in the following way. Let \( G(ij) \) denote the multigraph \( G \) but with one bond removed, \( N(i, j) \rightarrow N(i, j) - 1 \). If \( N(i, j) = 0 \) then we set \( G(ij) = 0 \). Further let \( G(G) \) and \( G(G(ij)) \) denote the respective symmetry groups. Then we define

\[
G' = \sum_{i<j} N(i,j) G(ij) \frac{|G(G)|}{|G(G(ij))|}.
\]

(48)

One has, so to speak, to break each bond of the multigraph and to sum over all results. Further, one has to introduce factors which compensate for the possible change of symmetries. For example, \( \Delta' = 6 \Delta + \cdots \). It is obvious that the evaluation of \( G' \) just yields \( \left. \frac{\partial}{\partial \alpha} G \right|_{\alpha=0} \). Then it is a straightforward task to calculate the magnetic moments \( \mu_0, \ldots, \mu_5 \) by using the above results for the \( t_n \). We will not, however, display these results and pass to the \( c_n \).

The coefficients of the high temperature expansion of \( \chi = \beta \frac{\text{Tr}(S^{(3)} \exp(-\beta H))}{\text{Tr}(\exp(-\beta H))} \) can be expressed through the \( \mu_n \) and the \( t_n \) which occur as coefficients of the series in the numerator or in the denominator, respectively. The first 6 coefficients are given by:

\[
\chi = \sum_{n=1}^{\infty} c_n \beta^n
\]
\[
= \mu_0 \beta - \mu_1 \beta^2 + \frac{1}{2} (\mu_2 - \mu_0 t_2) \beta^3 + \frac{1}{6} (t_3 \mu_0 + 3t_2 \mu_1 - \mu_3) \beta^4
\]
\[
+ \frac{1}{24} (6t_4 \mu_0 - t_4 \mu_0 - 4t_3 \mu_1 - 6t_2 \mu_2 + \mu_4) \beta^5
\]
\[
+ \frac{1}{120} (t_5 \mu_0 - 30t_2 \mu_1 + 5t_4 \mu_1 + 10t_3 \mu_3 + 10t_2 (-2t_3 \mu_0 + \mu_3) - \mu_5) \beta^6.
\]  

(50)
Inserting the known values for the $t_n$ and the $\mu_n$ yields the desired results for the $c_n$. Similarly as in section 3.2, a variety of product rules can be used to simplify the resulting expressions revealing the extensive character of the $c_n$. By this we mean the following. If the spin system under consideration would have a periodic lattice structure of, say, $K$ lattice units with periodic boundary conditions, it follows immediately that the evaluation of a single multigraph $\mathcal{G}$ linearly scales with $K$, and hence with $N$, as long as $\mathcal{G}$ is connected. For unconnected $\mathcal{G}$ the evaluation scales with $K^c$ where $c$ is the number of connected components of $\mathcal{G}$. Obviously, products of evaluations of connected multigraphs $\mathcal{G}_\nu \mathcal{G}_\mu$ would scale with $K^2$. It turns out that the elimination of these and higher products in the expression for the $c_n$ by means of the rules (4)-(21) also eliminates the evaluation terms of unconnected multigraphs. This has to be expected on physical grounds, since the total susceptibility of a spin lattice should be an extensive quantity, i.e. linearly scale with $K$. But it is an additional consistency test of our results that the non-extensive contributions to the $c_n$ actually cancel.

We will now represent the results for the susceptibility’s HTE up to sixth order in the inverse temperature $\beta$. $c_1$ and $c_2$ are well-known, $c_3$ has already been published in [3], but $c_4$, $c_5$ and $c_6$ seem to be new, although the polynomials which appear in these expressions are known up to 8th order, see [1].

\begin{align*}
  c_1 &= \frac{N r}{3}, \\
  c_2 &= -\frac{2}{9} r^2 \mathcal{G}_1, \\
  c_3 &= -\frac{1}{18} r^2 \mathcal{G}_2 + \frac{2}{27} r^3 \mathcal{G}_3, \\
  c_4 &= \frac{2}{135} r^2 (-1 + r + r^2) \mathcal{G}_4 + \frac{1}{54} r^3 \mathcal{G}_5 + \frac{1}{27} r^3 \mathcal{G}_7 - \frac{2}{81} r^4 \mathcal{G}_8, \\
  c_5 &= \frac{1}{648} r^2 (-3 + 6 r + 4 r^2) \mathcal{G}_9 - \frac{2}{405} r^3 (-1 + r + r^2) \mathcal{G}_{10} \\
  &\quad + \frac{1}{108} r^3 \mathcal{G}_{12} - \frac{1}{243} r^4 \mathcal{G}_{13} - \frac{1}{540} r^3 (-3 + 8 r + 8 r^2) \mathcal{G}_{14} \\
  &\quad - \frac{1}{486} r^4 \mathcal{G}_{15} - \frac{1}{162} r^4 \mathcal{G}_{16} - \frac{2}{243} r^4 \mathcal{G}_{19} - \frac{4}{243} r^4 \mathcal{G}_{21} + \frac{2}{243} r^5 \mathcal{G}_{22}, \\
  c_6 &= -\frac{1}{113400} r^2 (192 - 522 r - 677 r^2 + 240 r^3 + 160 r^4) \mathcal{G}_{23} \\
  &\quad - \frac{1}{1944} r^3 (-3 + 6 r + 4 r^2) \mathcal{G}_{24} - \frac{1}{972} r^3 (-3 + 3 r + 2 r^2) \mathcal{G}_{26} \\
  &\quad - \frac{1}{972} r^4 \mathcal{G}_{27} - \frac{1}{2430} r^3 (-6 + 21 r + 16 r^2) \mathcal{G}_{28} \\
  &\quad + \frac{1}{4860} r^4 (-3 + 8 r + 8 r^2) \mathcal{G}_{29} + \frac{2}{1215} r^4 (-1 + r + r^2) \mathcal{G}_{30} \\
  &\quad - \frac{1}{324} r^4 \mathcal{G}_{33} + \frac{1}{24300} r^3 (9 - 126 r - 12 r^2 + 152 r^3) \mathcal{G}_{34} - \frac{1}{648} r^4 \mathcal{G}_{35}.
\end{align*}
\begin{align}
&+ \frac{1}{1620} r^4 (-3 + 8r + 8r^2) \overline{G_{37}} - \frac{5}{972} r^4 \overline{G_{38}} + \frac{1}{729} r^5 \overline{G_{39}} \\
&+ \frac{1}{2430} r^4 (-7 + 12r + 12r^2) \overline{G_{42}} + \frac{1}{1458} r^5 \overline{G_{43}} - \frac{1}{648} r^4 \overline{G_{44}} \\
&+ \frac{1}{486} r^5 \overline{G_{45}} + \frac{2}{729} r^5 \overline{G_{50}} + \frac{1}{1620} r^4 (-1 + 16r + 16r^2) \overline{G_{51}} \\
&+ \frac{2}{729} r^5 \overline{G_{52}} + \frac{2}{729} r^5 \overline{G_{53}} + \frac{5}{729} r^5 \overline{G_{56}} - \frac{2}{729} r^6 \overline{G_{57}} .
\end{align}
Moments of Heisenberg Hamiltonians

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