Abstract

The evolution equation for the expectation values of the Boltzmann factor between valence bond states is evaluated in lowest order of the dimer cluster expansion. Explicit formulas are given for the internal energy and the specific heat of the $d$-dimensional antiferromagnetic Heisenberg model.
1. Introduction

A new approach to the spin $\frac{1}{2}$ quantum Heisenberg model with Hamiltonian:

$$H = \sum_{<x,y>} 4(x, y)$$

(1.1)

where:

$$(x, y) = \frac{1}{4}(1 - \vec{\sigma}(x)\vec{\sigma}(y))$$

(1.2)

has been proposed by one of us in the preceding paper [1], which is referred as paper 1 in the following. In this second paper we are going to exploit the new method in the sector with total spin 0. It was pointed out in paper 1, that the partition function in the spin 0 sector:

$$\text{tr} (\exp{\beta H_0}) = \frac{1}{a_0} \sum_K f(\beta, K)$$

(1.3)

contains already the whole information on the thermodynamics of the antiferromagnetic Heisenberg model in the absence of an external field – i.e. for vanishing magnetization $M = \frac{S}{V} = 0$. Moreover, it was shown that the partition function (1.3) is obtained from the expectation values of the Boltzmann factor $\exp(\beta H_0)$ between valence bond states $|K\rangle$:

$$f(\beta, K) = \langle K|\exp(\beta H_0)|K\rangle.$$ (1.4)

These expectation values were proven to obey an evolution equation:

$$\frac{\partial}{\partial \beta} f(\beta, K) = (dV + 3N_1(K)) f(\beta, K)$$

$$+ \sum_{<x,y>} (f(\beta, Q_+(x, y)K) - f(\beta, Q_-(x, y)K))$$

(1.5)

where $Q_{\pm}(x, y)$ are permutation operators which act on the valence bond configuration $K$, as defined in eqs.(2.13,14) of paper 1. $N_1(K)$ is the number of dimers. These are the nearest neighbour valence bonds on the configuration $K$.

It is clear from the evolution equation (1.5) that the expectation values $f(\beta, K)$ increase much stronger with $\beta$ on configurations with a large dimer density $x = \frac{N_1}{V}$. On the other hand, these configurations have low entropy, since the number of valence bond configurations $\nu(N_1, V)$ with a given number of dimers $N_1$ decrease as $(N_1!)^{-1}$. Therefore, if we assume that the averages:

$$f(\beta, N_1) = \frac{1}{\nu(N_1, V)} \sum_{K(N_1)} f(\beta, K(N_1))$$

(1.6)

over all valence bond configurations $K(N_1)$ with a fixed number $N_1$ of dimers behave in the combined limit:

$$V, N_1, n \rightarrow \infty, \quad x = N_1/V, \quad \beta \quad \text{fixed}$$

(1.7)

as:

$$f(\beta, N_1) = \exp(V\phi(\beta, x))$$

(1.8)
one is led to the conclusion that the zero density \((x = 0)\) contribution of the dimers determines the thermodynamical properties of the model. This statement holds in general provided that the function \(\phi(\beta, x)\) is differentiable with respect to \(x\). E.g. the internal energy per site at fixed inverse temperature \(\beta\) is given by:

\[
U(\beta) = \frac{\partial}{\partial \beta} \phi(\beta, x = 0).
\]  

We are not yet in the position to evaluate the exact evolution equation (1.5) in the thermodynamical limit. However it will be shown in section 2 that the lowest order in the ‘dimer cluster expansion’ can be solved analytically in the thermodynamical limit. Results for the ground-state energy and the specific heat of the AFH-model in dimensions \(d = 1, 2, 3\) are presented in sections 3 and 4.

2. The Dimer Cluster Expansion in the Spin 0 Sector

In paper \(1\) an approximation scheme was proposed for the evaluation of the evolution equation (1.5) in the thermodynamical limit. In lowest order of this ‘dimer cluster expansion’ (1.5) is averaged over all valence bond configurations \(K\) with a fixed number \(N_1(K)\) of dimers. The approximation would be exact if the right hand side of (1.5) could be expressed as well in terms of the averages (1.6). This is not possible for all the terms in the sum on the right hand side of (1.5). Here we approximate the \(f(\beta, K)\) by their average (1.6). The approximate evolution equation can be brought into the form:

\[
\frac{\partial}{\partial \beta} f(\beta, N_1) = (dV + 3N_1)f(\beta, N_1) + V \sum_j c_j(N_1, V)f(\beta, N_1 + j). \tag{2.1}
\]

In the combined limit (1.7) the coefficients \(c_j(N_1, V)\) were found to be (eqs(5.5-11) of paper \(1\)):

\[
\begin{align*}
c_{-2}(x) & = -w_1, \tag{2.2} \\
c_{-1}(x) & = 3w_1 - w_2 - 2(2d - 1)x, \tag{2.3} \\
c_0(x) & = -3w_1 + w_2 + 4(2d - 1)x - d + x, \tag{2.4} \\
c_1(x) & = w_1 - 2(2d - 1)x + d - x. \tag{2.5}
\end{align*}
\]

Here \(w_1(x)\) and \(w_2(x)\) are the probabilities to find on the valence bond configurations \(K(N_1)\) dimer pairs with arbitrary and parallel orientation, respectively. The approximate evolution equation (2.1) can be solved analytically in the combined limit (1.7) if we assume that the averages (1.6) have the form (1.8). Then eq.(2.1) yields a partial differential equation for \(\phi(\beta, x)\):

\[
\frac{\partial}{\partial x} \phi(\beta, x) = \log R \tag{2.6}
\]

\[
\frac{\partial}{\partial \beta} \phi(\beta, x) = L(x, R) \tag{2.7}
\]

where

\[
L(x, R) = d + 3x + \sum_j c_j(x)R^j \tag{2.8}
\]
with the initial condition:

\[ \phi(\beta = 0, x) = 0. \] (2.9)

The solution proceeds as follows. We first introduce \( R \) instead of \( \beta = \beta(x, R) \) as a new variable by means of the Legendre transform:

\[ \Phi(x, R) = \phi(\beta, x) - \beta \frac{\partial}{\partial \beta} \phi(\beta, x). \] (2.10)

Then we find for the partial derivatives:

\[ \left. \frac{\partial \Phi}{\partial x} \right|_R = \log R - \beta \frac{\partial}{\partial x} L(x, R), \] (2.11)

\[ \left. \frac{\partial \Phi}{\partial R} \right|_x = -\beta \frac{\partial}{\partial R} L(x, R). \] (2.12)

If we eliminate \( \beta \):

\[ \frac{\partial \Phi}{\partial R} \frac{\partial L}{\partial x} = \left( \frac{\partial \Phi}{\partial x} - \log R \right) \frac{\partial L}{\partial R}. \] (2.13)

we get a partial differential equation for \( \Phi(x, R) \) with initial condition:

\[ \Phi(x, R = 1) = 0. \] (2.14)

A solution of eqs. (2.13), (2.14) is easily found:

\[ \Phi(x, R) = x \log R - \int_1^R \frac{dR'}{R'} g(R', L(x, R)) \] (2.15)

provided that \( g(R', L(x, R)) \) solves the implicit equation:

\[ x = g(R' = R, L(x, R)). \] (2.16)

Therefore we get the integrand \( g(R, L) \) in eq. (2.15) from

\[ L(g, R) = L. \] (2.17)

3. Thermodynamical Properties in One Dimension

The probability \( w_1(x) \) to find dimer pairs on the valence bond configurations \( K(N_1) \) can be calculated analytically in the case \( d = 1 \), as is done in appendix A:

\[ w_1(x) = \frac{x^2}{1 - x}. \] (3.1)

The implicit equation (2.17) for \( g(R, L) \) turns out to be quadratic and can be easily solved:

\[ g_{\pm}(R, L) = 1 - \frac{1}{2a(R)} \left( L - b(R) \pm \sqrt{D(R, L)} \right) \] (3.2)

where

\[ a(R) = 4R - 11 + 5R^{-1} - R^{-2}, \] (3.3)
\[ b(R) = -4R + 14 - 8R^{-1} + 2R^{-2}, \quad (3.4) \]

\[ D(R, L) = (L - b(R))^2 - 4a(R) \frac{(R - 1)^3}{R^2}. \quad (3.5) \]

The solution has to satisfy eq.(2.16) which means in particular for:

\[ x = 0, \quad L(x = 0, R) = R, \quad g(R, L = R) = 0. \quad (3.6) \]

We have plotted in Fig.1 both solutions given by eq.(3.2). The condition (3.6) is satisfied for:

\[ g_+(R, L = R) = 0 \quad \text{if} \quad 1 < L < L_1 = 2.387425 \quad (3.7) \]

\[ g_-(R, L = R) = 0 \quad \text{if} \quad L_1 < L < L_2 = 2.588229. \quad (3.8) \]

Both solutions meet each other at \( R = R_2(L) \), which defines the zero of \( D(R, L) \). This zero produces a branch point singularity of \( g(R, L) \) in the complex \( R \)-plane, which has to be taken into account if we define the path of integration for the solution (2.15):

\[ \Phi(x, R) = x \log R - \int_1^R \frac{dR'}{R'} g_+(R', L) \quad \text{for} \quad L = L(x, R) < L_1 \quad (3.9) \]

\[ \Phi(x, R) = x \log R - \int_1^{R_2(L)} \frac{dR'}{R'} g_+(R', L) - \int_{R_2(L)}^R \frac{dR'}{R'} g_-(R', L) \quad (3.10) \]

for \( L_1 < L(x, R) < L_2 \).

Finally, we need the relation (2.12) for going back to the original variable, the inverse temperature \( \beta \):

\[ \beta(x, R) = R \int \frac{dR'}{R'} \frac{\partial}{\partial L} g_+(R', L) \quad \text{for} \quad L = L(x, R) < L_1 \quad (3.11) \]

\[ \beta(x, R) = \int_1^{R_2(L)} \frac{dR'}{R'} \frac{\partial}{\partial L} g_+(R', L) + \int_{R_2(L)}^R \frac{dR'}{R'} \frac{\partial}{\partial L} g_-(R', L) \quad (3.12) \]

for \( L_1 < L(x, R) < L_2 \).

Since \( R \) and \( L \) vary only in open and finite intervals:

\[ 1 < R < R_2(L_2) = 3.772126, \quad 1 < L < L_2 \quad (3.13) \]

the derivatives (2.6) and (2.7) are finite and the premise for eq.(1.9) is satisfied. Therefore the thermodynamical properties are obtained from the solution \( \phi(\beta, x) \) at vanishing dimer density:

\[ x = 0, \quad L = R = \frac{\partial}{\partial \beta} \phi(\beta, x = 0) = U(\beta). \quad (3.14) \]
The inverse temperature $\beta(U)$ as function of the internal energy $U$ can be taken from eqs.\((3.11,12)\) for \((x = 0, L = R = U)\). This function is shown in Fig.2. It develops a singularity for

$$R = U \rightarrow L_2, \ \ \beta \rightarrow \infty.$$  

(3.15)

which can be identified with the low temperature limit. Moreover we see from eq.\((1.9)\) that $L_2$ is just the ground state energy per site $h_0 = L_2 = 2.588229$. This value is 7\% below the exact value $h_0 = 4 \log 2$ which gives us an idea on the accuracy of the lowest order in the dimer cluster expansion. In Fig.3 we present the specific heat as function of the temperature.\(^\dagger\) Position and height of the maximum are:

$$T = 0.982(0.962) \ \ \ \ C = 0.296(0.350)$$  

(3.16)

For comparison we have listed in brackets the estimates of ref. [2], obtained from small rings up to 16 sites. The low temperature behavior [3] of the specific heat, as it is predicted by conformal invariance and derived rigorously by J. Suzuki, Y. Akutsu and M. Wadati:

$$C(T) = \frac{1}{3} T \ \ \ \ \text{for} \ \ \ T \rightarrow 0$$  

(3.17)

is represented in Fig.3 by the dotted line. The high temperature expansion has been computed to order 21 [4] and is represented in Fig.3 by the dashed line.

4. Thermodynamical Properties in Two and Three Dimensions

The probabilities $w_1(x)$, $w_2(x)$ to find on the valence bond configurations $K(N_1)$ dimer pairs with arbitrary and parallel orientation are determined in appendix A:

$$w_1(x) = (2d - 1)^2 \frac{x^2}{d - x}$$  

(4.1)

$$w_2(x) = 2(d - 1) \frac{x^2}{d - 2x}.$$  

(4.2)

The implicit equation \((2.17)\)-together with \((2.8)\) and \((2.2-5)\)- turns out to be of third order now:

$$g^3 a(R, d) + g^2 (b(R, d) - 2 \frac{L}{d^2}) + g (c(R, d) + 3 \frac{L}{d}) = L - dR$$  

(4.3)

where

$$a(R, d) = 2 \frac{(2d - 1)^2}{R^2 d^2} + \frac{1}{R d^2} (-24d^2 + 18d - 4) + \frac{1}{d^2} (24d^2 - 10d + 8) - 8R$$  

(4.4)

$$b(R, d) = -\frac{(2d - 1)^2}{R^2 d^2} + \frac{1}{d R} (12d^2 - 2d - 1) - \frac{1}{d} (12d^2 + 10d + 5) + 4R(d + 2)$$  

(4.5)

$$c(R, d) = \frac{2}{R} (1 - 2d) + 8d - R(4d + 2).$$  

(4.6)

\(^\dagger\)Our definition \((1.1)\) and \((1.3)\) of $H$ and $\beta$ differ from the usual one. Our $\beta$ is related to the usual definition of the temperature via: $\beta = (2dT)^{-1}$. 

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The real solutions \( g_{\pm}(R, L) \) are shown in Figs. 4 and 5 for \( d = 2 \) and \( d = 3 \), respectively. We observe that the condition (2.16) for \( x = 0, L(x = 0, R) = dR \):

\[
g_\sigma(R, L = dR) = 0, \quad \sigma = +, -
\]

is satisfied for the solution:

\[
\sigma = +: \quad \text{if} \quad 1 < L < L_1(d)
\]
\[
\sigma = -: \quad \text{if} \quad L_1(d) < L < L_2(d)
\]

where

\[
L_1(d = 2) = 3.625833, \quad L_2(d = 2) = 4.154262 \quad (4.10)
\]
\[
L_1(d = 3) = 4.862986, \quad L_2(d = 3) = 5.399962. \quad (4.11)
\]

Both solutions meet each other at \( R = R_2(L) \), where the derivative \( \frac{\partial g}{\partial R} \) diverges. At this point \( g(R, L) \) has a branch point singularity in the complex \( R \)-plane which we pick up in the path of integration for the solution (2.15). The thermodynamical properties of the AFH model in \( d \) dimensions are obtained from:

\[
\beta(x = 0, R) = \int_{R_1}^{R} \frac{dR'}{R'} \frac{\partial}{\partial L} g_+(R', L) \quad \text{for} \quad L = dR < L_1 \quad (4.12)
\]

\[
\beta(x = 0, R) = \int_{R_2(dR)}^{R} \frac{dR'}{R'} \frac{\partial}{\partial L} g_+(R', L) + \int_{R_2(dR)}^{R} \frac{R^m}{R'} \frac{\partial}{\partial L} g_-(R', L) \quad \text{for} \quad L_1 < dR < L_2. \quad (4.13)
\]

This function relates the inverse temperature \( \beta \) with the internal energy per site:

\[
U(\beta) = \frac{\partial}{\partial \beta} \phi(\beta, x = 0) = L = dR
\]

which is shown in Fig.6 for \( d = 2 \) and \( d = 3 \). A singularity appears for:

\[
dR \to L_2, \quad \beta(0, R) \to \infty \quad (4.15)
\]

i.e. in the zero temperature limit. \( L_2 \) is the groundstate energy per site in the lowest order of the dimer cluster expansion (cf.(2.1)). The values listed in eqs. (4.10,11) have to be compared with the estimates of ref.[5,6,7] for the groundstate energy per site \( e(d) \):

\[
h_0(d = 2) = 2 - 4e(d = 2) = 4.678, \quad h_0(d = 3) = 3 - 4e(d = 3) = 6.611 \quad (4.16)
\]

The specific heats for \( d = 2 \) and \( d = 3 \) are shown in Figs.7 and 8, respectively. For \( d = 2 \) the low temperature behavior is known from chiral perturbation theory [8]:

\[
C(T) = \left( \frac{6\zeta(3)}{\pi c^2} \right) T^2 \quad \text{for} \quad T \to 0 \quad (4.17)
\]
where
\[ c = 1.68 \quad (4.18) \]
is the spin wave velocity \[5\].
The high temperature expansion has been computed up to order 10 for \( d = 2 \) \[9\] and \( d = 3 \) \[10\]. The high and low temperature limits are represented in Fig.7 by the dashed and dotted curves. We observe good agreement in the high temperature regime, whereas the low temperature behavior (4.17) cannot be reproduced by the lowest order of the dimer cluster expansion.

5. Summary and Perspectives

In this paper we have started a first attempt to evaluate the evolution equation (1.5) for the expectation values (1.4) of the Boltzmann factor between valence bond states. To lowest order in the dimer cluster expansion the thermodynamical limit of the evolution equation (2.1) leads to a partial differential equation (2.6-7) which can be solved analytically up to integrations. As a result, we obtain an explicit representation (3.11-12, 4.12-13) of the inverse temperature \( \beta \) as function of the internal energy per site \( U \) for the antiferromagnetic Heisenberg model in dimensions \( d = 1, 2, 3 \). The predictions of the lowest order in the dimer cluster expansion for the specific heat are in agreement with the high temperature expansion but they are in disagreement with the low temperature expansion (3.17) and (4.17). This means, that the formation of dimer clusters-which has not been taken into account in the lowest order approximation (2.1)- plays an important role for the correct description of the low temperature behavior. The specific heat has a maximum at temperatures \( T(d) \) which decreases with the dimension \( d \). The height of the maxima is almost independent of \( d \), the width shrinks with \( d \). Therefore, we do not see any indications for a phase transition in our results for the specific heat in three dimensions, as it was suggested from the high temperature expansion of ref.[10].
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Appendix

A Dimer Pairs on Valence Bond Configurations

In this appendix we will compute the probability:

\[ w([1,2][3,4]) = \nu(N_1)^{-1} \sum_{K(N_1)} \delta([1,2][3,4] \in K(N_1)) \]  \hspace{1cm} (A1)

to find a dimer pair at the neighbouring sites 2 and 3 on a valence bond configuration \( K(N_1) \) with \( N_1 \) dimers. \( \nu(N_1) \) denotes the total number of these configurations.

Let us keep the \( N_1 \) dimers fixed in a ‘dimer configuration’ \( D(N_1) \) and ask how many possibilities we have to connect the remaining \( V - 2N_1 \) sites on the lattice by valence bonds. This number is approximately given by \((V - 2N_1 - 1)!!\) i.e. by the total number of valence bond configurations on the remaining sites. In a strict sense we should count only those configurations on the remaining sites which do not contain any further dimers. Indeed these configurations dominate the thermodynamical limit, since configurations with dimers have lower entropy. This argument tells us that the dimer probability (A.1) on the valence bond configuration \( K(N_1) \) is just the same as on the dimer configuration \( D(N_1) \):

\[ w([1,2][3,4]) = \rho(N_1, V)^{-1} \sum_{D(N_1)} \delta([1,2],[3,4] \in D(N_1)) \]  \hspace{1cm} (A2)

where:

\[ \rho(N_1, V) = \sum_{D(N_1)} \]  \hspace{1cm} (A3)

is the number of possibilities to distribute \( N_1 \) dimers on a lattice with \( V \) sites.

For \( d = 1 \) and open boundary conditions one finds:

\[ \rho_o(N_1, V) = \frac{(V/2 + n_1)!}{(2n_1)!(V/2 - n_1)!} \]  \hspace{1cm} (A4)

where \( n_1 = V - 2N_1 \) is the number of sites which are not occupied with dimers.

For \( d = 1 \) and periodic boundary conditions one finds:

\[ \rho(N_1, V) = \rho_o(N_1, V) + \rho_o(N_1 - 1, V - 2) - \rho_o(N_1 + 1, V - 2). \]  \hspace{1cm} (A5)

The second and third term take into account the different interpretation of the valence bond \([1,V]\). It is a dimer for periodic but not for open boundary conditions.

In the case \( d = 1 \) the probability (A.3) to find a dimer pair turns out to be:

\[ w([1,2][3,4]) = \frac{\rho_o(N_1 - 2, V - 4)}{\rho(N_1, V)} \]  \hspace{1cm} (A6)

which leads in the combined limit (1.7) to eq.(3.1).

In the case \( d = 2 \) and \( d = 3 \) the dimer pair probability (A.2) can be determined in a simulation of the monomer dimer system. We have done that on the lattices \( \square \).

\footnote{The simulations on the 200\(^3\) lattice has been performed on the connection Machine CM5. The results are based upon a test version of the software where the emphasis was on providing functionality. This software release has not had the benefit of optimization or performance.}
The results for the dimer pair probabilities \( w_l(x), l = 1, 2 \) together with the fits (4.1-2) are shown in Fig. 9 for \( d = 2 \) and in Fig. 10 for \( d = 3 \). The behavior of \( w_1(x) \) for \( x = N_1/V \to 0 \) and \( x \to 1/2 \) and that of \( w_2(x) \) for \( x \to 0 \) can be easily checked by combinatorical considerations. Note that the fit (4.1) for the dimer pair probability \( w_1(x) \) is perfect for \( d = 2 \) and \( d = 3 \). We therefore believe, that (4.1) represents indeed the exact formula for this quantity. On the other hand, the fit (4.2) for the parallel dimer pair probability \( w_2(x) \) is not perfect. We therefore expect that the exact formula for this quantity is more complicated than the fit (4.2).
Figure Captions

1. The real solutions (3.2) of the implicit equations (2.17) for \( d = 1 \). The solutions coincide on the solid curve \( R = R_2(L) \) where the square root in eq. (3.2) vanishes.

2. The inverse temperature \( \beta(U) \) versus the internal energy per site \( U \), as it follows from (3.11,12) for \( x = 0, U = L = R, d = 1 \).

3. The specific heat of the one-dimensional AFH-model in lowest order of the dimer cluster expansion. The dotted curve represents the low temperature behavior (3.17), the dashed curve the high temperature expansion of ref.[4].

4. The real solutions \( g_{\pm}(R; L) \) of the implicit equation (4.3) for \( d = 2 \). The solutions coincide on the solid curve \( R = R_2(L) \).

5. Same as Fig.4 for \( d = 3 \).

6. The inverse temperature \( \beta(U) \) versus the internal energy per site \( U \) as it follows from eqs. (4.12,13) for \( x = 0, U = L = dR \). Solid curve: \( d = 2 \), dotted curve: \( d = 3 \).

7. The specific heat of the \( d = 2 \) AFH model in lowest order of the dimer cluster expansion. The dotted curve represents the low temperature behavior (4.17); the dashed curve the high temperature expansion of ref.[9].

8. Same as Fig.7 for \( d = 3 \).

9. The dimer pair probabilities for \( d = 2 \): solid curve: \( w_1(x) \), dotted curve: \( w_2(x) \)

10. Same as Fig.9 for \( d = 3 \).