Spin Hartree-Fock approach to quantum Heisenberg antiferromagnets in low dimensions

A. Werth,1 P. Kopietz,1,2 and O. Tsyplatyev1

1Institut für Theoretische Physik, Universität Frankfurt, Max-von-Laue Strasse 1, 60438 Frankfurt, Germany
2Department of Physics and Astronomy, University of California, Irvine, CA, 92697, USA

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We construct a new mean-field theory for quantum (spin-1/2) Heisenberg antiferromagnet in one (1D) and two (2D) dimensions using a Hartree-Fock decoupling of the four-point correlation functions. We show that the solution to the self-consistency equations based on two-point correlation functions does not produce any unphysical finite-temperature phase transition in accord with Mermin-Wagner theorem, unlike the common approach based on the mean-field equation for the order parameter. The next-neighbor spin-spin correlation functions, calculated within this approach, reproduce closely the strong renormalization by quantum fluctuations obtained via Bethe ansatz in 1D and a small renormalization of the classical antiferromagnetic state in 2D. The heat capacity approximates with reasonable accuracy the full Bethe ansatz result at all temperatures in 1D. In 2D, we obtain a reduction of the peak height in the heat capacity at a finite temperature that is accessible by high-order 1/T expansions.

Interest in the low-dimensional quantum antiferromagnets has been revived in the last decades by the discovery of the high-Tc superconductors, where the physics of the quantum spin fluctuations on a square lattice was suggested to be the main mechanism behind superconductivity.1 More recently, the magnetic properties of insulators such as Cs2CuCl4 2,3, CsNiCl3 4, Cs2CuBr4 5, where at low temperatures a moderate degree of anisotropy (about 0.3 − 0.4) makes their dimensionality intermediate between one and two, have caused a new resurgence of activity in this problem. In both cases the dimensionality is smaller than three, where the classical long-range order in the ground state was rigorously proven6,7, but is bigger than strictly one, making the exact Bethe ansatz solution8 inapplicable. Thus, a more accurate description of the effect of quantum fluctuations is required, which become strong in reduced dimensions and for the quantum spin S = 1/2.

A popular method to deal with low-dimensional quantum spin systems is Takahashi’s modified spin-wave theory that was quite successful especially for ferromagnets, where it, for instance at low temperature, reproduces correctly subleading terms of the free energy9 obtained using the thermodynamic Bethe ansatz approach10,11. Generally, this and other predictions of the Takahashi’s theory are almost equivalent to the Schwinger-boson mean-field theory formulated by Arovas and Auerbach12 and to the one-loop renormalization group calculations13. However, at high temperature the spin-wave result for the free energy is divergent9 disagreeing entirely with the high temperature expansion in its limit of validity. In the antiferromagnetic case predictions of the modified spin-wave theory are not as good for S = 1/2. In 1D, they lead to a gapful ground state and an exponential two-point correlation function at zero temperature that deviates strongly from the known from Bethe ansatz gapless ground state8 and algebraic correlations14,17 at zero temperature. Also, in both 1D and 2D, there is a spurious finite temperature phase transition within the spin-wave approach, which is explicitly forbidden in these dimensions by the Mermin-Wagner theorem18. The latter problem stems from the need of introducing two sublattices in the construction of the spin-wave theory in the antiferromagnetic case12,19, which is based on the simplest mean-field approximation using the sublattice magnetization (a one-point correlation function) as the order parameter and causes an order-disorder phase transition in all dimensions that is not washed out by spin waves.

In this paper we construct an alternative mean-field approach for the spin-1/2 antiferromagnet in 1D and 2D based on the decoupling of the four-point correlation functions. The corresponding self-consistency equations are derived using the Hartree-Fock decoupling for the Heisenberg interactions and assuming the exclusive statistics of free magnons. It recovers almost all effects of the strong renormalisation of the classical spin picture in 1D at low temperature established by Bethe ansatz, including the heat capacity and the static correlation functions, with the most notable exception of the logarithmic contribution to the magnetic susceptibility that is driven by the low-energy physics of Luttinger liquid and requires taking into account even higher order correlation functions. At high temperature our method recreates the 1/T expansion and produces no phase transition at intermediate temperatures. In 2D the same approach recovers only a small renormalisation of the classical antiferromagnetic state20 in the next-neighbor spin-spin correlation function and the high temperature expansion, producing again no finite temperature phase transition. The height of a smooth peak (instead of a transition) at an intermediate temperature, for instance in the heat capacity, is reduced in 2D with respect its value in 1D that is still accessible via high order 1/T expansion in 2D21,22 and is already captured qualitatively on the level of the two-point correlation functions. The biggest quantitative
discrepancy of ignoring three- and higher-point correlation functions occurs at intermediate temperatures and is of the order of 20% in 1D, where the thermodynamic quantities can be calculated at arbitrary temperatures \cite{23,26} using the thermodynamic Bethe ansatz \cite{10,11}.

We study Heisenberg model for spin-1/2 in the presence of an external magnetic field, \( B \), in one (\( D = 1 \)) and two (\( D = 2 \)) dimensions.

\[
H = B \sum_{\mathbf{r}} S^z_{\mathbf{r}} + \frac{J}{2} \sum_{\mathbf{r},\mathbf{\delta}} S_\mathbf{r} \cdot S_{\mathbf{r}+\mathbf{\delta}},
\]  

(1)

where \( J \) is the exchange energy, \( S^z_{\mathbf{r}} = S^z_{\mathbf{r}} \pm iS^y_{\mathbf{r}} \) are the spin-1/2 operators at site \( \mathbf{r} \), the sum over \( \mathbf{r} \) runs over equidistant (square) lattice consisting of \( N = L^D \) spins in 1D (2D), and sum over \( \mathbf{\delta} \) runs over 2 or 4 nearest-neighbors in the corresponding dimension. Below we impose periodic boundary conditions, \( S_{\mathbf{r}+\mathbf{\gamma}} = S_\mathbf{r} \), restrict ourselves to the antiferromagnetic exchange energy, \( J > 0 \), and use the units where \( g\mu_B = 1 \).

Before proceeding with solving the model in Eq. (1), we reduce the number of the spin components in it by utilizing the following spin-1/2 identity \( S^\pm_{\mathbf{r}} = S^x_{\mathbf{r}} \pm iS^y_{\mathbf{r}} = \frac{1}{2} (S^+_{\mathbf{r}} \pm iS^-_{\mathbf{r}}) \). This turns the Zeeman term in the Hamiltonian into a quadratic form and the \( z \) component of the scalar product into a quartic form, expressing Eq. (1) in terms of only \( S^\pm_{\mathbf{r}} \) operators.

In the Fourier domain, \( S^\pm_{\mathbf{r}} = N^{-1/2} \sum_k S^\pm_k e^{\pm i k \cdot \mathbf{r}} \), the resulting Hamiltonian becomes a sum of a quadratic and a quartic form in the single spin operators,

\[
H = \sum_k \left( B - DJ + \varepsilon_k \right) S^+_k S^-_k \\
+ \frac{1}{N} \sum_{k_1, k_2, k_3, k_4} \delta_{k_1+k_2+k_3+k_4} \delta_{k_3-k_4} \delta_{k_1+k_2} \delta_{k_3+k_4} \langle S^+_k S^-_k S^+_k S^-_k \rangle,
\]  

(2)

where the dispersion is \( \varepsilon_k = J \sum_{\alpha} \cos k_\alpha \), the sum \( \sum_{\alpha} \) contains only one term \( \alpha = x \) in 1D and it runs over two spatial dimensions, \( \sum_{\alpha=x,y} \) in 2D, and the sum over momentum, \( \sum_k \), also runs over one \( (k) \) or two \( (k_x, k_y) \) components of the wave vector in the corresponding dimension.

In order to analyze the model in Eq. (2) we assume that its eigenstates factorize in the momentum domain, \( i.e. \) they can be approximated by product states of single magnon excitations in the thermodynamic limit \cite{27}. At a finite temperature this approach corresponds to writing down the following product density matrix: \( \rho = \prod_k |m_k \rangle \langle k| + (1 - m_k) \rangle \), where \( |k\rangle \) is a single magnon state at a given \( k \), exclusive statistics for the states with different \( k \) is implied \cite{30}, \( m_k \) are scalar parameters, and the normalisation is chosen as \( \text{Tr} \rho = 1 \).

We believe that this density matrix gives a close enough approximation to the many-magnon states. The expectation value of the Hamiltonian in Eq. (2) with respect to this \( \rho \) gives the energy of the system, \( E = \langle H \rangle \), as a function of parameters \( m_k \).

\[
E = \sum_k \left( B - DJ + \varepsilon_k \right) m_k - \frac{1}{N} \sum_{k_1, k_2} \varepsilon_{k_1-k_2} m_{k_1} m_{k_2},
\]  

(3)

where the contribution of the terms with \( k_1 = k_2 \) in the second line vanishes in the \( N \to \infty \) limit and the average of an operator is \( \langle \ldots \rangle = \text{Tr} \rho \ldots \). The second term in Eq. (3) is equivalent to the Hartree-Fock approximation to the quartic interaction term in Eq. (2). \( \langle S^+_k S^-_k S^+_k S^-_k \rangle \approx m_k m_k \delta_{k_1,k_2} \delta_{k_3,k_4} + m_k (1 - m_k) \delta_{k_1,k_4} \delta_{k_1,k_2} \), where the first term is the direct and the second is the exchange part.

The average of the operator \( S^+_k S^-_k \) in the first term in Eq. (2) gives the scalar parameter \( \langle S^+_k S^-_k \rangle = m_k \) that can be interpreted as a two-point correlation function. The inverse Fourier transform gives the correlation function \( \sum_k e^{-i k \cdot \mathbf{r}} m_k / N = \langle S^+_0 S^-_0 \rangle \), where \( 0 \) is a reference point on the lattice in 1D and 2D and the translational invariance of the model in Eq. (1) was used.

The values of the mean-field parameters \( m_k \) at a finite temperature \( T \) can be found in the usual way by minimizing the free energy, \( F = E - TS \), with respect to them. The energy \( E \) is given by Eq. (3) and the von Neumann entropy, \( S = -k_B \text{Tr} \rho \ln \rho \), is given by \(-k_B \sum_k (m_k \ln m_k + (1 - m_k) \ln (1 - m_k)) \), where \( k_B \) is the Boltzmann constant. Solving \( \partial F / \partial m_k = 0 \) we obtain the mean-field self-consistency equations as

\[
m_k = \frac{1}{e^{\beta (B-2DJ)} + 1},
\]  

(4)

where \( \beta = 1 / (k_B T) \) is the inverse temperature. The above is a large set of \( N \) non-linear equations for the mean-field parameters \( m_k \). However, the \( m_k \) enter in
the exponential function only under a sum. Thus, the number of the independent non-linear equations can be reduced greatly. We introduce $1 + D$ extensive variables as $s = \sum \alpha m_k/N - 1/2$ and $u_\alpha = -\sum \alpha m_k \cos k_\alpha/N + 1/2$, where $u_\alpha = u$ is a scalar in 1D and $u_\alpha = (u_x, u_y)$ is a vector in 2D. Substituting these definitions into Eq. (4) we express its the right-hand-side in terms of only $s$ and $u_\alpha$ and then substituting the resulting expressions for $m_k$ back into the definitions for $s$ and $u_\alpha$ we rewrite Eq. (4) as a set of only $1 + D$ independent equations,

$$s = \int \frac{d^Dk}{(2\pi)^D} \frac{1}{e^{\beta(B/2+2DJs+2J\sum \alpha u_\alpha \cos k_\alpha)}+1} - \frac{1}{2},$$  

(5)

$$u_\alpha = \frac{1}{2} - \int \frac{d^Dk}{(2\pi)^D} \frac{\cos k_\alpha}{e^{\beta(B/2+2DJ\sum \alpha u_\alpha \cos k_\alpha)}+1},$$  

(6)

where the sum over $k$ was turned into an integral in the thermodynamic limit as $\sum_k/N \rightarrow \int d^Dk/(2\pi)^D$. Here the parameter $s$ gives the average magnetization per spin as $\sum \alpha (\langle s^2 \rangle)^{1/2}/N = s$ and the parameter $u_\alpha$ is related to the kinetic energy of magnons.

There is only one non-trivial solution of Eqs. (5, 6). Let us analyze it at $B = 0$. At zero temperature the integrands are proportional to the Heaviside step function, $\lim_{\beta \rightarrow \infty} \exp(\beta x) + 1^{-1} = \Theta(-x)$, then the integrals can be calculated explicitly, and we obtain $s = 0$ (unpolarized ground state) and $u_x = u_y = 1/2 + D/\pi^2$. On the other hand, at high temperature, the exponential expands into a Taylor series in $\beta \ll 1$ up to the leading order as $\exp(\beta x) + 1^{-1} = 1/2 + O(\beta)$ and we get $s = 0$ and $u_x = u_y = 1/2$. At intermediate temperatures the equations can be solved numerically.

The thermodynamic quantities can be expressed through solutions of Eqs. (5, 6) at different temperatures and magnetic fields. The energy in Eq. (5) can be written as a function of $s$ and $u_\alpha$ using their definitions in terms of $m_k$: $E = N(Bs + DJs^2 - J\sum \alpha u_\alpha^2)$. From which, using the basic definition of the heat capacity we obtain

$$\frac{C}{N} = \frac{1}{N} \frac{\partial E}{\partial T} = (B + 2DJs) \frac{\partial s}{\partial T} - 2J \sum \alpha u_\alpha \frac{\partial u_\alpha}{\partial T}. $$  

(7)

The temperature dependence of $C$ in 1D and in 2D (at $B = 0$) is plotted in Fig. 1. In 1D we can compare our result with the full quantum mechanical result obtained via the thermodynamic Bethe ansatz machinery in Refs. [10, 11] in Refs. [23, 24, 25]. Up to the intermediate temperatures Eqs. (5, 6) agree quite well with it including the linear dependence of $C$ at low temperatures. Eqs. (5, 6) also reproduce the correctly coefficient of the leading term of the $1/T$ expansion at high temperatures. However, in the intermediate temperature region, from $T \gtrsim J/2$, the difference, see the black solid and the red dash-dotted lines in Fig. 1 is still appreciable, up to 20%. In 2D the available high order $1/T$ expansion [25] covers a significant temperature range down to the peak, which amplitude is reduced with respect to the 1D case. The result of solving Eq. (7), the blue dashed line in Fig. 1, gives about the same discrepancy of up to 20% with [21] in the intermediate temperature region.

This discrepancy can be understood in term of improving approximate description of the Heisenberg model by taking into account higher order correlation functions. The usual way of introducing the mean-field approximation to the model in Eq. (1) is retaining only the one-point correlation functions, $\langle S^\alpha_z \rangle = \pm m$, where $m$ is the order (a single mean-field) parameter and ± describes even/odd sublattice of the antiferromagnet. Neglecting the quadratic terms in fluctuations around $\langle S^\alpha_z \rangle$ (and assuming that $\langle S^\alpha_s \rangle = 0$) in Eq. (1), the usual self-consistency equations are the same for each sublattice for $B = 0$.

$$2m = \tanh(\beta DJm).$$  

(8)

This equation does predict the antiferromagnetic order at $T = 0$, but it also introduces an erroneous phase transition at a finite $T$ in low dimensions, which is explicitly forbidden by the Mermin-Wagner theorem [18]. In the present work we take into account two-point correlation function solving the self-consistency equations in Eq. (1) for $N$ mean-field parameters $m_k$. This approach contains more information about the quantum fluctuations,

![](image.png)

Figure 2. The static correlation function $\langle S_0 \cdot S_r \rangle$ in 1D evaluated by solving the self-consistency equation in Eqs. (9, 10) and using Eqs. (9, 10).

The main plot is the temperature dependence of the correlation length $\xi$ in the exponential regime $r > r_*$ obtained numerically (full circles) and the $1/T$ result of Bethe ansatz (black line). The inset is the correlation function for an intermediate temperature $T = 0.01J$ obtained numerically (open circles); the zero temperature result, $1/r$, is valid in the short-range region $r < r_*$ (dashed red line) and an exponential, $\exp(-r/\xi)$, is valid in the long-range region $r > r_*$ (solid blue line).
which play a stronger role in low dimensions, improving the approximation qualitatively, i.e., not introducing a finite $T$ phase transition, and quantitatively, as illustrated in 1D by comparison with the Bethe ansatz in Fig. 4. An approach that accounts for higher than two-point correlation functions would improve the accuracy even further.

Another thermodynamic quantity that is of interest in magnets is the magnetic susceptibility, $\chi = \partial (\sum_r (S^x_r)) / \partial B$. Using as before the identity $S^x_r = S^z_r S^z_r - 1/2$ and the definition of $s$ in terms of $m_k$, we obtain $\chi = N \partial s / \partial B$. The temperature dependence of this result at $B = 0$ shows a better (in comparison with the more crude approximation in Eq. (8)) agreement with the full Bethe ansatz calculation [23, 24], both quantitatively and qualitatively. However, there are larger deviations at small temperatures, unlike for the heat capacity, due to the logarithmic corrections [25]. They are essentially an effect of Luttinger physics manifesting hydrodynamic modes which are not captured on the level of the two-point correlation functions in Eq. (4).

The static correlation functions can also be calculated in terms of the solutions of Eqs. (5,6). Expressing the operator $S_0 \cdot S_r$ in the Fourier domain and evaluating its finite temperature average using $\langle S_0 \cdot S_r \rangle$ in 1D, established by Bethe ansatz, and only a small correction in the two-dimensional antiferromagnet is known to have an exponential dependence on temperature, $\xi \propto \exp (\text{const}/T)$, [36]. Numerically we find that the result of Eqs. (5,10) is consistent with [36] at a small temperature range below $T \simeq J$, which is still accessible due to not so large values of $r_s$ at relatively not so low temperatures.

In conclusion, we have constructed a new mean-field approach based on two-point correlation functions for spin-1/2 antiferromagnet in 1D and 2D, for which the effect of quantum fluctuations is the strongest. Solutions of the corresponding self-consistency equations recover the strong renormalisation of the classical spin picture in 1D, established by Bethe ansatz, and only a small correction to the classical antiferromagnet in 2D. This approach produces no finite temperature phase transitions in accord with the Mermin-Wagner theorem and the 1/T-expansion at high temperature in $D = 1$ and $D = 2$. The biggest quantitative discrepancy of ignoring three- and higher-point correlation functions occurs at intermediate temperatures and is up to $\sim 20\%$ that can be assessed in 1D, where the thermodynamic quantities can be calculated at arbitrary temperatures using the thermodynamic Bethe ansatz. The controversy about the effect of dimensionality in the anisotropic 2D quantum antiferromagnets, e.g., Cs$_2$CuCl$_4$ (the ratio of the exchange constants is $J_L/J_\parallel \simeq 0.33$) for which neutron scattering shows both signatures of one-dimensional physics [37], and a dispersion in the perpendicular direction [38], can be explained here as a dimensional crossover, where strong effects of quantum fluctuations in 1D disappear smoothly as the coupling between the chains is increased.

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