INTERNAL ENERGY OF HEISENBERG SPIN-1/2 J₁ - J₂ ANTIFERROMAGNET ON THE BODY-CENTERED-CUBIC LATTICE IN TYABLIKOV APPROXIMATION

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Abstract: Magnetic properties of spin ½ J₁-J₂ quantum Heisenberg antiferromagnet on body centered cubic lattice are investigated in the paper. By using two-time temperature Green's functions, sublattice magnetization and critical temperature depending on the frustration ratio J₂/J₁ are obtained in both stripe and Neel phase. The analysis of ground state sublattice magnetization and internal energy indicates the first order phase transition from Neel to stripe phase for 0.7 < J₂/J₁ < 0.8, which is in agreement with previous studies.

Keywords: Heisenberg J₁ - J₂ antiferromagnet, internal energy, Neel and stripe phase, Tyablikov approximation.

1. INTRODUCTION

Frustrated spin systems [1] represent a dynamic area of condensed matter physics, offering possibilities for theoretical as well as experimental research. As a rule, competing interactions yield rich phase diagram and spectrum of elementary excitations [2] and such structures are interesting by themselves. The most famous examples include J₁-J₂ Ising and Heisenberg models on a square lattice [3,2]. In both cases, the phase diagram displays strong dependence on the frustration ratio p = J₂/J₁. For J₂ < J₁, localized spins exhibit standard Neel-type of order, while for J₂ > J₁/2 a new phase, the so called stripe phase, emerges. A common feature of these 2D models is the equal number of sublattices in Neel and stripe phase.

The discovery of high-temperature superconductors based on iron compounds [4,5] provided additional stimulus and pointed on somewhat more complicated models. The one considered in the present paper is spin ½ Heisenberg antiferromagnet on the body centered cubic (bcc) lattice with the nearest and next-nearest neighbor interactions J₁ and J₂. Its model Hamiltonian is compactly written as

\[ \hat{H} = J₁ \sum_{\langle i,j \rangle} S_i \cdot S_j + J₂ \sum_{\langle \langle i,j \rangle \rangle} S_i \cdot S_j, \]

where the first sum, \( \langle i, j \rangle \), captures \( z₁ = 8 \) nearest neighbours, while the second one \( \langle \langle i, j \rangle \rangle \) picks up \( z₂ = 6 \) next-nearest neighbors. The mean field calculation [6] indicates the existence of two phases, as shown in Figure 1. The Neel phase (AF1) can be described by a standard two-sublattice system as in the case of 2D models, while the collinear phase (AF2) can be properly described only with four sublattices. The mean field theory also predicts \( p_{MF} = J₂ / J₁ = 2/3 \) as the critical value for the frustration ratio [7].

More sophisticated approaches were also applied to the model defined in (1). Schmidt et al. [8] performed exact diagonalization of finite 3D lattices with periodic boundary conditions (for \( N > 36 \)) and found the discontinuity in ground state energy at \( J₂ / J₁ = 0.693 \) indicating a first order quantum transition between two phases. This is confirmed by calculation of the sublattice magnetization and extrapolation to infinite lattice. Oitmaa and Zhang [7] performed high-order linked-cluster expansion at \( T = 0K \) and concluded that two branches of ground state energy for two phases cross for \( J₂ / J₁ = 0.705 \pm 0.005 \).

Finally, Majumdar and Datta [9] presented a non-linear spin-wave theory (up to quartic terms in Bose-operators) and found similar results. Majumdar [10] also extended this problem to the antiferromagnet on stacked square lattices with different exchange in vertical direction.

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The aim of this paper is to present the first calculation within spin operator Green’s functions formalism. As described in Section 2, it allows one to obtain all the quantities necessary for the analysis of phase transitions at $T = 0K$. Finally, Section 3 is devoted to the numerical analysis. Throughout the paper „h.c.” denotes „hermitian conjugate” and we have set $\hbar = k_B = 1$.

2. RANDOM PHASE APPROXIMATION FOR SPIN GREEN’S FUNCTIONS

We will now analyze the system for $S = 1/2$ using the formalism of two-time temperature dependent Green’s functions (GF) [11-16] the use of which allowed us to calculate all necessary correlators. For the application of GFs technique on Heisenberg AFMs, see e.g. [17-19]. Retarded GF will be defined as

$$G_{m,n}(t,t') = \langle \langle \hat{A}_n(t) | \hat{B}_m(t') \rangle \rangle = \theta(t-t') \langle [\hat{A}_n(t), \hat{B}_m(t')] \rangle$$

(2)

where $\theta(t-t')$ denotes the Heaviside step function.

In our case operators $\hat{A}$ and $\hat{B}$ will be the spin operators located at a particular site $n(m)$ belonging to the sublattice $\alpha : S^\alpha_i (i = x, y, z, +, -)$. Following the standard procedure, we write down the equations

$$\langle [\hat{S}^\alpha_\beta (\alpha) | \hat{B}_m (\gamma) ] \rangle \approx \langle [\hat{S}^\alpha_\beta (\alpha) ] \langle [\hat{B}_m (\gamma) ] \rangle$$

(3)

where $\hat{S}^+$ and $\hat{S}^-$ are standard spin rising and lowering operators and operator $\hat{B}$ will be chosen in a convenient way later (see [13,14] for more details). Due to translational invariance within each of the sublattices, $[\hat{S}^\alpha_\beta (\alpha) ] = \sigma(\alpha)$ does not depend on site.

After decoupling, the system of equations for GFs can be closed by performing spatial and temporal Fourier-transform

$$\frac{1}{N} \sum_{n=-N}^{N} e^{ik(n-m)} \int d(t-t') \int e^{i\omega(t-t')} \langle [\hat{S}^\alpha_\beta (\alpha) | \hat{B}_m (\gamma) ] \rangle$$

(4)

where $n$ denotes the site in the given sublattice. $\hat{A}_i$ connects the given site to its $z_1 (8)$ nearest neighbors. $\hat{A}_2$ connects each ion to its $z_2 (6)$ next nearest neighbors belonging to the same sublattice. We have performed the rotation of the quantization axis in one of the sublattices. Both exchange parameters $(J_{1}, J_{2})$ are assumed to be positive. The coefficient $1/2$ in front of $J_{2}$ takes care of the possible double summing of the term within the same sublattice. The distance between NNN will be denoted by $\alpha$ (not to be confused with the index of a sublattice).

The first step will be to write the equations of motion for two operators $\hat{S}^\alpha_\alpha (\alpha), \hat{S}^\alpha_\beta (\alpha)$:

$$\langle [\hat{S}^\alpha_\beta (\alpha) | \hat{B}_m (\gamma) ] \rangle$$

(5)
The internal energy of the system is obtained by using equations of motion (6) together with two additional equations corresponding to $a \leftrightarrow b$. We multiply them with the suitable operators and combine them with the identities valid for $S = 1/2$. The averaging of this expression yields the internal energy...
gy in terms of correlation functions of only two op-
erators, in this way avoiding any decoupling proce-
12.

\[
\langle \hat{H}_{AF1} \rangle = \frac{J_1}{4} \sum_{n,a} \left\langle \hat{S}_n^z(a) \hat{S}_{n+a_1}^z(b) + h.c. \right\rangle + \frac{J_2}{8} \sum_{n,a_2} \left\langle \hat{S}_n^z(a) \hat{S}_{n+a_2}^z(a) + h.c. \right\rangle + \frac{J_2}{8} \sum_{n,a_2} \left\langle \hat{S}_n^z(b) \hat{S}_{n+a_2}^z(b) + h.c. \right\rangle
\]

\[
- \frac{1}{4} \sum_n \left\langle \hat{S}_n^z(a) \frac{d\hat{S}_n^z(a)}{dt} + h.c. \right\rangle + \frac{1}{4} \sum_n \left\langle \hat{S}_n^z(b) \frac{d\hat{S}_n^z(b)}{dt} + h.c. \right\rangle
\]

\[
- \frac{J_1}{4} \sum_{n,a_i} \left\langle \hat{S}_n^z(a) \hat{S}_{n+a_i}^z(b) + h.c. \right\rangle + \frac{J_2}{4} \sum_{n,a_2} \left\langle \hat{S}_n^z(a) + \hat{S}_n^z(b) \right\rangle
\]

(19)

Moving on to spatial and temporal Fourier trans-
forms, one can evaluate all necessary correla-
tion functions, leading to

\[
\langle \hat{H}_{AF1} \rangle = -\frac{\sigma_0}{2N} \sum_k \gamma_{2k}^2 + p \frac{\sigma_0}{2N} \sum_k \gamma_{2k}^2 \left[ 1 - p(1 - \gamma_{2k}) \right] + \frac{\sigma_0^2}{N} \sum_k \left\{ \omega_k - [1 - p(1 - \gamma_{2k})] - \frac{\sigma_0}{2} (1 - p) \right\}
\]

(20)

with \( \sigma_0 \) defined by (18). These results will be ana-
lyzed further on.

The Hamiltonian of the system can be written in the following form:

\[
\hat{H}_{AF2} = J_1 \sum_{n,a_i} \left\{ \hat{S}_n^z(a_i) \hat{S}_{n+a_i}^z(a_i) + \hat{S}_n^z(a_2) \hat{S}_{n+a_2}^z(a_3) \right\} + J_1 \sum_{n,a_i} \left\{ \hat{S}_n^z(a_1) \hat{S}_{n+a_1}^z(a_4) + \hat{S}_n^z(a_3) \hat{S}_{n+a_3}^z(a_4) \right\}
\]

(21)

We are now dealing with four sublattices (\( a_1 \)
to \( a_4 \)) and \( n \) implies the site of the corresponding
lattice. It is important to notice that while summation
over second neighbours (\( \lambda_2 \)) is the same as in the
previous section, there are two summations over the
nearest neighbours. Summation over \( \lambda_1 \) covers the
following four neighbours (\( a/2, a/2 \), \( -a/2, a/2 \),
\( -a/2, -a/2 \), \( a/2, -a/2 \)), while the summation over \( \lambda_1^f \)
covers \( -a/2, -a/2, -a/2, a/2 \), \( a/2, a/2, -a/2, a/2 \).

For this reason we will define two Fourier transforms \( \gamma_k \) and \( \gamma_k^* \).

Since both of them are complex numbers, they are
actually complex conjugate to each other. (Please
note that \( \gamma_1 \) from the previous section is the sum of
these two, so it is a real number.)

The explicit expression which takes into ac-
count the rotation of quantization axes is

\[
\hat{H}_{AF2} = J_1 \sum_{n,a_i} \left\{ \frac{1}{2} \left[ \hat{S}_n^z(a_i) \hat{S}_{n+a_i}^z(a_i) + h.c. \right] - \hat{S}_n^z(a_4) \hat{S}_{n+a_i}^z(a_4) \right\}
\]

\[
+ J_1 \sum_{n,a_i} \left\{ \frac{1}{2} \left[ \hat{S}_n^z(a_1) \hat{S}_{n+a_1}^z(a_1) + h.c. \right] - \hat{S}_n^z(a_3) \hat{S}_{n+a_2}^z(a_3) \right\}
\]

\[
+ J_1 \sum_{n,a_i} \left\{ \frac{1}{2} \left[ \hat{S}_n^z(a_2) \hat{S}_{n+a_2}^z(a_2) + h.c. \right] - \hat{S}_n^z(a_3) \hat{S}_{n+a_3}^z(a_3) \right\}
\]

\[
+ J_2 \sum_{n,a_i} \left\{ \frac{1}{2} \left[ \hat{S}_n^z(a_1) \hat{S}_{n+a_1}^z(a_2) + h.c. \right] - \hat{S}_n^z(a_4) \hat{S}_{n+a_2}^z(a_4) \right\}
\]

\[
+ J_2 \sum_{n,a_i} \left\{ \frac{1}{2} \left[ \hat{S}_n^z(a_2) \hat{S}_{n+a_2}^z(a_2) + h.c. \right] - \hat{S}_n^z(a_3) \hat{S}_{n+a_3}^z(a_3) \right\}
\]

(22)

Writing down four equations of motion for GF:

\[
G_1 = \left\langle \left\langle \hat{S}_n^z(a_1) \right\rangle \right\rangle_{k,E}, \ G_2 = \left\langle \left\langle \hat{S}_n^z(a_2) \right\rangle \right\rangle_{k,E}, \ G_3 = \left\langle \left\langle \hat{S}_n^z(a_1) \right\rangle \right\rangle_{k,E}, \ G_4 = \left\langle \left\langle \hat{S}_n^z(a_3) \right\rangle \right\rangle_{k,E}
\]

(23)

invoking the RPA with equal average sublattice magnetization \( \sigma \) and performing the spatial Fourier
giving four magnon branches. The phase is calculated as described in Section 2.1. The evaluation for magnon energies: 

\[ 0^2 2 4 \]

transforms, one can write the following set of equations for GFs

\[
(E - 6\alpha J_2)G_i - \alpha J_2\gamma_{i2k}G_2 - \alpha J_1\gamma_{i1k}G_3 - \alpha J_1\gamma_{i1k}G_4 = \frac{i}{2\pi}\left(\hat{\mathcal{S}}^i(a_i), \hat{B}\right) \]

\[
\alpha J_2\gamma_{i2k}G_1 + (E + 6\alpha J_2)G_2 + \alpha J_1\gamma_{i1k}G_3 + \alpha J_1\gamma_{i1k}G_4 = \frac{i}{2\pi}\left(\hat{\mathcal{S}}^i(a_i), \hat{B}\right) \]

\[
-\alpha J_1\gamma_{i1k}G_1 - \alpha J_1\gamma_{i1k}G_2 + (E - 6\alpha J_2)G_3 - \alpha J_2\gamma_{i2k}G_4 = \frac{i}{2\pi}\left(\hat{\mathcal{S}}^i(a_i), \hat{B}\right) \]

\[
\alpha J_1\gamma_{i1k}G_1 + \alpha J_1\gamma_{i1k}G_2 + \alpha J_2\gamma_{i2k}G_3 + (E + 6\alpha J_2)G_4 = \frac{i}{2\pi}\left(\hat{\mathcal{S}}^i(a_i), \hat{B}\right) \]

This set leads to the following biquadratic equation for magnon energies:

\[ E^4 - 2\alpha E^2 + B = 0 \]

with

\[ A = \alpha^2 J_2^2(z_1^2 - \gamma_{i2k}^2), B = \alpha^4 \left[J_1^2(z_1^2 - \gamma_{i2k}^2)^2 - J_1^4(\gamma_{i1k}^2 - \gamma_{i1k}^2)^2 - 4J_1^2J_2^2 \right|6\gamma_{i1k} - \gamma_{i1k}\gamma_{i2k}] \]

\[ z_1 = 4, z_2 = 6 \]

giving four magnon branches

\[ E_{12k} = \pm\sqrt{A - \sqrt{A^2 - B}}, E_{34k} = \pm\sqrt{A + \sqrt{A^2 - B}}. \]

These can be also written as

\[ E_{1k} = \alpha J_1 \left[ \frac{J_2}{J_1} \right]^2 (z_1^2 - \gamma_{i2k}^2) + K, \]

\[ E_{3k} = \alpha J_1 \left[ \frac{J_2}{J_1} \right]^2 (z_2^2 - \gamma_{i2k}^2) - K, \]

\[ E_{2k} = -E_{1k}, E_{4k} = -E_{3k}, \quad K = \left(\gamma_{i1k}^2 - \gamma_{i1k}^2\right)^2 + 4\left[ \frac{J_2}{J_1} \right] \left|6\gamma_{i1k} - \gamma_{i1k}\gamma_{i2k}\right|^2 \]

Choosing Green’s functions for convenient notation in AF2 phase operators, we can calculate the sublattice magnetiza-

\[ \sigma = \left[ \frac{J_2}{J_1} \sum_k \frac{1}{K} \frac{6K + 12 |\gamma_{i1k}|^2 - \gamma_{i2k}^2 (\gamma_{i1k}^2 + \gamma_{i1k}^2)}{\coth \frac{E_{1k}}{2T}} + \frac{6K - 12 |\gamma_{i1k}|^2 + \gamma_{i2k}^2 (\gamma_{i1k}^2 + \gamma_{i1k}^2)}{\coth \frac{E_{1k}}{2T}} \right]^{-1} \]

The internal energy (per lattice site) in AF2 phase is calculated as described in Section 2.1. The final result is

\[ \langle \hat{H}_{AF2} \rangle_{J_iN} = \sigma_0 \sum_k \frac{-2K |\gamma_{i1k}|^2 + (\gamma_{i1k}^2 - \gamma_{i2k}^2)^2 - 12p^2 (\gamma_{i1k}^2 + \gamma_{i1k}^2)\gamma_{2k} + 4p^2 |\gamma_{i1k}|^2 \gamma_{2k}}{K \cdot K_i} \]

\[ + \frac{6K - 12 |\gamma_{i1k}|^2 + \gamma_{i2k}^2 (\gamma_{i1k}^2 + \gamma_{i1k}^2)}{\coth \frac{E_{1k}}{2T}} \]

\[ + \frac{\gamma_{i1k}^2 - \gamma_{i1k}^2}{K \cdot K_i} \]

\[ + \frac{2 |\gamma_{i1k}|^2 (K + 72 p^2) - 12p^2 (\gamma_{i1k}^2 + \gamma_{i1k}^2)\gamma_{2k}}{K \cdot K_i} \]

\[ + \frac{\gamma_{i1k}^2 - \gamma_{i1k}^2}{K \cdot K_i} \]

\[ + \frac{6 |\gamma_{i1k}|^2 (K + 72 p^2) + 12p^2 (\gamma_{i1k}^2 + \gamma_{i1k}^2)\gamma_{2k}}{K \cdot K_i} \]

\[ + \frac{2 |\gamma_{i1k}|^2 - 6\gamma_{i1k}^2 + 6 (\gamma_{i1k}^2 + \gamma_{i1k}^2) - 2 \gamma_{i1k}^2}{K \cdot K_i} \]
\[
+ \frac{\sigma^2}{N} \sum_i \left[ K_i + K_i - 12p \right] - 6p \sigma_0 
\]

with \( \sigma_0 \) defined by (29) and

\[
K_i = \left( \frac{J_i}{J_1} \right)^2 (z_i^2 - \gamma_{i3}) + K, \quad K_i = \left( \frac{J_i}{J_1} \right)^2 (z_i^2 - \gamma_{i3}) - K
\]

and \( p = \frac{J_2}{J_1} \).

3. RESULTS AND DISCUSSION

Numerical solutions of equations for sublattice magnetization AF1 and AF2 phase are shown in Figure 2 (See also [20]). As expected, the next-nearest neighbor coupling reduces the sublattice magnetization in AF1 phase, eventually destroying the long range order at \( p = \frac{J_2}{J_1} \approx 0.65 \). It is also seen that the stripe long range order emerges at \( p \approx 0.7 \). Since the magnon energies (in RPA) are proportional to sublattice magnetization, our analysis suggests that elementary excitations may not be well defined around \( p \approx 0.7 \). However, GF method (within RPA) alone cannot resolve whether or not a transition from the Neel order to the spin-liquid state occurs or the system directly passes to the stripe phase.

![Figure 2](image-url)

**Figure 2.** a) Ground state magnetization and b) internal energy of frustrated spin \( \frac{1}{2} \) Heisenberg antiferromagnet on bcc lattice. Dashed line (for \( p > 0.65 \)) denotes extrapolation.

Similar conclusions are drawn from the plot of the ground state energy (see Figure 2). We see that the transition from Neel to stripe order is predicted to take place at \( p \approx 0.8 \). This value is somewhat higher than the one obtained from the analysis of the sublattice magnetization and the Neel temperature [20]. Still, it is higher than the mean field result and quite close to the values obtained by other methods (see discussion in [20] and references therein).

Finally, it is safe to say that RPA GF method yields results in agreement with nonlinear spin-wave theory and linked cluster expansions. Its main advantage is direct applicability to the ground state (\( T = 0K \)) and higher temperatures (the vicinity of Neel temperature) so that reliable results may be obtained with a single set of parameters in wide temperature range.

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5. REFERENCES


