Original scientific papers UDK 621.318:66
doi: 10.7251/COMEN1402190K

INTERNAL ENERGY OF HEISENBERG SPIN-1/2 J_1 - J_2 ANTIFERROMAGNET ON THE BODY-CENTERED-CUBIC LATTICE IN TYABLIKOV APPROXIMATION

Darko Kapor, Petar Mali, Milan Pantić, Milica Pavkov Hrvojević, Slobodan Radošević, Milica Rutonjski*
University of Novi Sad, Faculty of Sciences, Department of Physics,
Trg Dositeja Obradovića 4, 21000 Novi Sad

Abstract: Magnetic properties of spin ½ J_1-J_2 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 J_2/J_1 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 $0.7 < J_2/J_1 < 0.8$, which is in agreement with previous studies.

Keywords: Heisenberg J_1 - J_2 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 J_1-J_2 Ising and Heisenberg models on a square lattice [3,2]. In both cases, the phase diagram displays strong dependence on the frustration ratio $p = J_2/J_1$. For $J_2 \ll J_1$, localized spins exhibit standard Neel-type of order, while for $J_2 > J_1/2$ 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 J_1 and J_2. Its model Hamiltonian is compactly written as

$$\hat{H} = J_1 \sum_{\langle i,j \rangle} S_i \cdot S_j + J_2 \sum_{\langle\langle i,j \rangle\rangle} S_i \cdot S_j \,, \qquad (1)$$

where the first sum, $\langle i,j \rangle$, captures $z_1 = 8$ nearest neighbours, while the second one $\langle\langle i,j \rangle\rangle$ picks up $z_2 = 6$ 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 $p_{\mathrm{MF}} = J_2 / J_1 = 2/3$ 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 $J_2 / J_1 = 0.693$ 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 $J_2 / J_1 = 0.705 \pm 0.005$.

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.

* Corresponding author: mpantic@df.uns.ac.rs

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 $\hbar = k_B = 1$.

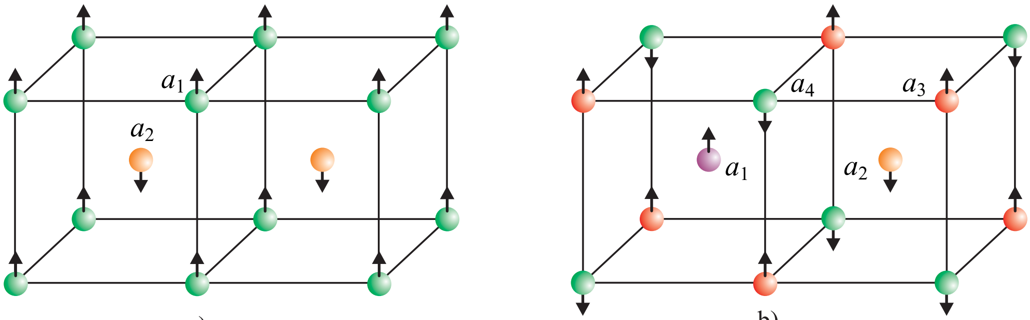

Figure 1. Body-centered cubic lattice in a) Neel (AF1) and b) stripe (AF2) phase

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

$$G_{n,m}(t,t') = \left\langle\left\langle \hat{A}_n(t) \,|\, \hat{B}_m(t') \right\rangle\right\rangle = \theta(t-t')\left\langle [\hat{A}_n(t), \hat{B}_m(t')] \right\rangle \tag{2}$$

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 α : $S_n^i(\alpha)(i = x, y, z, +, -)$. Following the standard procedure, we write down the equations of motion for GFs. However, the infinite chain of equations for GFs is produced in this manner. One way of truncating the chain in the lowest order is to apply the so-called Tyablikov's decoupling or Random Phase Approximation (RPA) in the following manner:

$$\left\langle\left\langle \hat{S}_n^z(\alpha)\hat{S}_l^i(\beta) \,|\, \hat{B}_m(\gamma) \right\rangle\right\rangle \cong \left\langle \hat{S}_n^z(\alpha) \right\rangle \left\langle\left\langle \hat{S}_l^i(\beta) \,|\, \hat{B}_m(\gamma) \right\rangle\right\rangle \tag{3}$$

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, $\left\langle \hat{S}_n^z(\alpha) \right\rangle = \sigma(\alpha)$ does not depend on site. After decoupling, the system of equations for GFs can be closed by performing spatial and temporal Fourier-transform

$$\left\langle\left\langle \hat{S}_n^i(\beta) \,|\, \hat{B}_m(\gamma) \right\rangle\right\rangle_{k,\omega} = \frac{1}{N}\sum_{n-m} e^{ik(n-m)} \int d(t-t') e^{i\omega(t-t')} \left\langle\left\langle \hat{S}_n^i(\beta,t) \,|\, \hat{B}_m(\gamma,t') \right\rangle\right\rangle \quad . \tag{4}$$

Here N is the total number of sites in the sublattice, while the wave vector k from reciprocal lattice is restricted to the first Brillouin zone.

2.1. AF1 phase

We start with the Hamiltonian of the system with two sublattices, a and b:

$$\hat{H}_{AF1} = J_1 \sum_{n,\lambda_1} \left\{ \frac{1}{2}\left[\hat{S}_n^+(a)\hat{S}_{n+\lambda_1}^+(b) + h.c.\right] - \hat{S}_n^z(a)\hat{S}_{n+\lambda_1}^z(b) \right\}$$
$$+ \frac{J_2}{2} \sum_{n,\lambda_2} \left\{ \frac{1}{2}\left[\hat{S}_n^+(a)\hat{S}_{n+\lambda_2}^-(a) + h.c.\right] + \hat{S}_n^z(a)\hat{S}_{n+\lambda_2}^z(a) \right\} + (a \to b) \tag{5}$$

Here n denotes the site in the given sublattice. λ_1 connects the given site to its z_1 (8) nearest neighbours. λ_2 connects each ion to its z_2 (6) next nearest neighbours 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 a (not to be confused with the index of a sublattice).

The first step will be to write the equations of motion for two operators $\hat{S}_n^+(a), \hat{S}_n^-(b)$:

$$i\frac{d\hat{S}_n^+(a)}{dt} = J_1\sum_{\lambda_1}\left(\hat{S}_n^z(a)\hat{S}_{n+\lambda_1}^-(b) + \hat{S}_n^+(a)\hat{S}_{n+\lambda_1}^z(b)\right) + J_2\sum_{\lambda_2}\left(\hat{S}_n^z(a)\hat{S}_{n+\lambda_2}^+(a) - \hat{S}_n^+(a)\hat{S}_{n+\lambda_2}^z(a)\right) \tag{6}$$

$$i\frac{d\hat{S}_n^-(b)}{dt} = -J_1\sum_{\lambda_1}\left(\hat{S}_n^z(b)\hat{S}_{n+\lambda_1}^+(a) + \hat{S}_n^-(b)\hat{S}_{n+\lambda_1}^z(a)\right) - J_2\sum_{\lambda_2}\left(\hat{S}_n^z(b)\hat{S}_{n+\lambda_2}^-(a) - \hat{S}_n^+(b)\hat{S}_{n+\lambda_2}^z(a)\right) \tag{7}$$

This enables us to write down the equations of motion for corresponding two GF, where $\hat{B}_m$ can be any suitably chosen spin operator.

$$E\left\langle\left\langle \hat{S}_n^+(a) \mid \hat{B}_m\right\rangle\right\rangle = \frac{i}{2\pi}\left\langle[\hat{S}_n^+(a),\hat{B}_m]\right\rangle + J_1\sum_{\lambda_1}\left(\left\langle\left\langle \hat{S}_n^z(a)\hat{S}_{n+\lambda_1}^-(b) \mid \hat{B}_m\right\rangle\right\rangle + \left\langle\left\langle \hat{S}_n^+(a)\hat{S}_{n+\lambda_1}^z(b) \mid \hat{B}_m\right\rangle\right\rangle\right) \tag{8}$$

$$+ J_2\sum_{\lambda_2}\left(\left\langle\left\langle \hat{S}_n^z(a)\hat{S}_{n+\lambda_2}^+(a) \mid \hat{B}_m\right\rangle\right\rangle - \left\langle\left\langle \hat{S}_n^+(a)\hat{S}_{n+\lambda_2}^z(a) \mid \hat{B}_m\right\rangle\right\rangle\right)$$

$$E\left\langle\left\langle \hat{S}_n^-(b) \mid \hat{B}_m\right\rangle\right\rangle = \frac{i}{2\pi}\left\langle[\hat{S}_n^-(b),\hat{B}_m]\right\rangle - J_1\sum_{\lambda_1}\left(\left\langle\left\langle \hat{S}_n^z(b)\hat{S}_{n+\lambda_1}^+(a) \mid \hat{B}_m\right\rangle\right\rangle + \left\langle\left\langle \hat{S}_n^-(b)\hat{S}_{n+\lambda_1}^z(a) \mid \hat{B}_m\right\rangle\right\rangle\right) \tag{9}$$

$$- J_2\sum_{\lambda_2}\left(\left\langle\left\langle \hat{S}_n^z(b)\hat{S}_{n+\lambda_2}^-(b) \mid \hat{B}_m\right\rangle\right\rangle - \left\langle\left\langle \hat{S}_n^+(b)\hat{S}_{n+\lambda_2}^z(b) \mid \hat{B}_m\right\rangle\right\rangle\right)$$

After performing RPA (3) and Fourier-transforms (4), one obtains:

$$\left[E - \left(z_1J_1\sigma(b) - z_2J_2\sigma(a) + z_2J_2\sigma(a)\gamma_{2k}\right)\right]\left\langle\left\langle \hat{S}^+(a) \mid \hat{B}\right\rangle\right\rangle_{k,E} - z_1J_1\sigma(a)\gamma_{1k}\left\langle\left\langle \hat{S}^-(b) \mid \hat{B}\right\rangle\right\rangle_{k,E} = \frac{i}{2\pi}\left\langle\left[\hat{S}^+(a),\hat{B}\right]\right\rangle_{k,E} \tag{10}$$

$$z_1J_1\sigma(b)\gamma_{1k}\left\langle\left\langle \hat{S}^+(a) \mid \hat{B}\right\rangle\right\rangle_{k,E} + \left[E + \left(z_1J_1\sigma(b) - z_2J_2\sigma(a) + z_2J_2\sigma(a)\gamma_{2k}\right)\right]\left\langle\left\langle \hat{S}^-(b) \mid \hat{B}\right\rangle\right\rangle_{k,E} = \frac{i}{2\pi}\left\langle\left[\hat{S}^-(b),\hat{B}\right]\right\rangle_{k,E} \tag{11}$$

The geometrical factors introduced in (10) and (11) are

$$\gamma_{1k} = \frac{1}{z_1}\sum_{\lambda_1}e^{ik\cdot\lambda_1} = \cos\frac{k_xa}{2}\cos\frac{k_ya}{2}\cos\frac{k_za}{2},\ \gamma_{2k} = \frac{1}{z_2}\sum_{\lambda_2}e^{ik\cdot\lambda_2} = \frac{1}{3}\left(\cos k_xa + \cos k_ya + \cos k_za\right) \tag{12}$$

Due to the rotation, one can assume that $\sigma(a) = \sigma(b) = \sigma$. (Actually, one can calculate sublattice magnetizations and then prove that they are equal.) Introducing the notation,

$$\varepsilon_1 = \sigma\left(J_1(0) - J_2(0) + J_2(k)\right), J_i(0) = z_iJ_i, J_i(k) = z_iJ_i\gamma_{ik}, i = 1,2 \tag{13}$$

the system (10) and (11) is rewritten as

$$\left(E - \varepsilon_1\right)\left\langle\left\langle \hat{S}^+(a) \mid \hat{B}\right\rangle\right\rangle_{k,E} - \sigma J_1(k)\left\langle\left\langle \hat{S}^-(b) \mid \hat{B}\right\rangle\right\rangle_{k,E} = \frac{i}{2\pi}\left\langle\left[\hat{S}^+(a),\hat{B}\right]\right\rangle_{k,E} \tag{14}$$

$$\sigma J_1(k)\left\langle\left\langle \hat{S}^+(a) \mid \hat{B}\right\rangle\right\rangle_{k,E} + \left(E + \varepsilon_1\right)\left\langle\left\langle \hat{S}^-(b) \mid \hat{B}\right\rangle\right\rangle_{k,E} = \frac{i}{2\pi}\left\langle\left[\hat{S}^-(b),\hat{B}\right]\right\rangle_{k,E}$$

Vanishing determinant of the system gives the Green's functions poles (the positive one defining the magnon energy)

$$E_{1/2}(k) = \pm E_k,\quad E_k = z_1J_1\sigma\sqrt{\left[1 - p(1-\gamma_{2k})\right]^2 - \gamma_{1k}^2},\quad p = \frac{z_2J_2}{z_1J_1} \tag{15}$$

so choosing $\hat{B}$ to be $\hat{S}_n^-(b)$, one obtains GF

$$G^{aa}(k,E) = \frac{i}{2\pi}\frac{\sigma}{E_k}\left[\frac{E_k + \varepsilon_1}{E - E_k} + \frac{E_k - \varepsilon_1}{E + E_k}\right] \tag{16}$$

Now the spectral theorem [12] gives:

$$\sigma = \frac{1}{2} - \frac{1}{N}\sum_k\left\langle \hat{S}^-\hat{S}^+\right\rangle_{k,E} = \frac{1}{2}\left(\frac{1}{N}\sum_k\frac{\varepsilon_1}{E_k}\coth\frac{E_k}{2T}\right)^{-1} \tag{17}$$

For $T = 0K$, we have

$$\sigma_0 = \frac{1}{2}\left(\frac{1}{N}\sum_k\frac{1 - p(1-\gamma_{2k})}{\sqrt{\left[1 - p(1-\gamma_{2k})\right]^2 - \gamma_{1k}^2}}\right)^{-1} \tag{18}$$

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 in terms of correlation functions of only two operators, in this way avoiding any decoupling procedure [12].

$$\begin{aligned}\left\langle \hat{H}_{AF1}\right\rangle &= \frac{J_1}{4}\sum_{n,\lambda_1}\left\langle \hat{S}_n^+(a)\hat{S}_{n+\lambda_1}^+(b)+h.c.\right\rangle + \frac{J_2}{8}\sum_{n,\lambda_2}\left\langle \hat{S}_n^+(a)\hat{S}_{n+\lambda_2}^-(a)+h.c.\right\rangle + \frac{J_2}{8}\sum_{n,\lambda_2}\left\langle \hat{S}_n^+(b)\hat{S}_{n+\lambda_2}^-(b)+h.c.\right\rangle \\ &-\frac{1}{4}\sum_n\left\langle \hat{S}_n^-(a)i\frac{d\hat{S}_n^+(a)}{dt}+h.c.\right\rangle + \frac{1}{4}\sum_n\left\langle \hat{S}_n^-(b)i\frac{d\hat{S}_n^+(b)}{dt}+h.c.\right\rangle \\ &-\frac{J_1}{4}\sum_{n,\lambda_1}\left\langle \hat{S}_{n+\lambda_1}^z(a)+\hat{S}_{n+\lambda_1}^z(b)\right\rangle + \frac{J_2}{4}\sum_{n,\lambda_2}\left\langle \hat{S}_{n+\lambda_2}^z(a)+\hat{S}_{n+\lambda_2}^z(b)\right\rangle\end{aligned} \tag{19}$$

Moving on to spatial and temporal Fourier transforms, one can evaluate all necessary correlation functions, leading to

$$\frac{\left\langle \hat{H}_{AF1}\right\rangle}{z_1J_1N} = -\frac{\sigma_0}{2N}\sum_k\frac{\gamma_{2k}^2}{\omega_k} + p\frac{\sigma_0}{2N}\sum_k\frac{\gamma_{2k}}{\omega_k}[1-p(1-\gamma_{2k})] + \frac{\sigma_0^2}{N}\sum_k\{\omega_k-[1-p(1-\gamma_{2k})]\} - \frac{\sigma_0}{2}(1-p) \tag{20}$$

with σ_0 defined by (18). These results will be analyzed further on.

2.2 AF2 phase

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

$$\begin{aligned}\hat{H}_{AF2} &= J_1\sum_{n,\lambda_1^a}\left[\hat{S}_n(a_1)\cdot\hat{S}_{n+\lambda_1^a}(a_4)+\hat{S}_n(a_2)\cdot\hat{S}_{n+\lambda_1^a}(a_3)\right] + J_1\sum_{n,\lambda_1^f}\hat{S}_n(a_1)\cdot\hat{S}_{n+\lambda_1^f}(a_3) \\ &+ J_1\sum_{n,\lambda_1^f}\hat{S}_n(a_2)\cdot\hat{S}_{n+\lambda_1^f}(a_4) + J_2\sum_{n,\lambda_2}\left[\hat{S}_n(a_1)\cdot\hat{S}_{n+\lambda_2}(a_2)+\hat{S}_n(a_3)\cdot\hat{S}_{n+\lambda_2}(a_4)\right]\end{aligned} \tag{21}$$

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 (λ_2) is the same as in the previous section, there are two summations over the nearest neighbours. Summation over λ_1 covers the following four neighbours $(a/2,a/2,a/2)$, $(-a/2,-a/2,a/2)$, $(-a/2,a/2,-a/2)$, $(a/2,-a/2,-a/2)$, while the summation over λ_1^f covers $(-a/2,-a/2,-a/2)$, $(a/2,a/2,-a/2)$, $(a/2,-a/2,a/2)$, $(-a/2,a/2,a/2)$. For this reason we will define two Fourier transforms $\tilde{\gamma}_k$ and $\tilde{\gamma}_k^*$. Since both of them are complex numbers, they are actually complex conjugate to each other. (Please note that γ_k from the previous section is the sum of these two, so it is a real number.)

The explicit expression which takes into account the rotation of quantization axes is

$$\begin{aligned}\hat{H}_{AF2} &= J_1\sum_{n,\lambda_1^a}\left\{\frac{1}{2}\left[\hat{S}_n^+(a_1)\hat{S}_{n+\lambda_1^a}^+(a_4)+h.c.\right]-\hat{S}_n^z(a_1)\hat{S}_{n+\lambda_1^a}^z(a_4)\right\} \\ &+ J_1\sum_{n,\lambda_1^f}\left\{\frac{1}{2}\left[\hat{S}_n^+(a_1)\hat{S}_{n+\lambda_1^f}^-(a_3)+h.c.\right]+\hat{S}_n^z(a_1)\hat{S}_{n+\lambda_1^f}^z(a_3)\right\} + J_1\sum_{n,\lambda_1^a}\left\{\frac{1}{2}\left[\hat{S}_n^+(a_2)\hat{S}_{n+\lambda_1^a}^+(a_3)+h.c.\right]-\hat{S}_n^z(a_2)\hat{S}_{n+\lambda_1^a}^z(a_3)\right\} \\ &+ J_1\sum_{n,\lambda_1^f}\left\{\frac{1}{2}\left[\hat{S}_n^+(a_2)\hat{S}_{n+\lambda_1^f}^-(a_4)+h.c.\right]+\hat{S}_n^z(a_2)\hat{S}_{n+\lambda_1^f}^z(a_4)\right\} \\ &+ J_2\sum_{n,\lambda_2}\left\{\frac{1}{2}\left[\hat{S}_n^+(a_1)\hat{S}_{n+\lambda_2}^+(a_2)+h.c.\right]-\hat{S}_n^z(a_1)\hat{S}_{n+\lambda_2}^z(a_2)+\frac{1}{2}\left[\hat{S}_n^+(a_3)\hat{S}_{n+\lambda_2}^-(a_4)+h.c.\right]-\hat{S}_n^z(a_3)\hat{S}_{n+\lambda_2}^z(a_4)\right\}\end{aligned} \tag{22}$$

Writing down four equations of motion for GF:

$$G_1 \equiv \left\langle\left\langle \hat{S}^+(a_1)\,|\,\hat{B}\right\rangle\right\rangle_{k,E},\ G_2 \equiv \left\langle\left\langle \hat{S}^-(a_2)\,|\,\hat{B}\right\rangle\right\rangle_{k,E},\ G_3 \equiv \left\langle\left\langle \hat{S}^+(a_3)\,|\,\hat{B}\right\rangle\right\rangle_{k,E},\ G_4 \equiv \left\langle\left\langle \hat{S}^-(a_4)\,|\,\hat{B}\right\rangle\right\rangle_{k,E} \tag{23}$$

invoking the RPA with equal average sublattice magnetization σ and performing the spatial Fourier

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

$$(E-6\sigma J_2)G_1-\sigma J_2\gamma_{2k}G_2-\sigma J_1\gamma_{1k}^*G_3-\sigma J_1\gamma_{1k}G_4=\frac{i}{2\pi}\left\langle\left[\hat{S}^+(a_1),\hat{B}\right]\right\rangle$$

$$\sigma J_2\gamma_{2k}G_1+(E+6\sigma J_2)G_2+\sigma J_1\gamma_{1k}G_3+\sigma J_1\gamma_{1k}^*G_4=\frac{i}{2\pi}\left\langle\left[\hat{S}^-(a_2),\hat{B}\right]\right\rangle \tag{24}$$

$$-\sigma J_1\gamma_{1k}G_1-\sigma J_1\gamma_{1k}^*G_2+(E-6\sigma J_2)G_3-\sigma J_2\gamma_{2k}G_4=\frac{i}{2\pi}\left\langle\left[\hat{S}^+(a_3),\hat{B}\right]\right\rangle$$

$$\sigma J_1\gamma_{1k}^*G_1+\sigma J_1\gamma_{1k}G_2+\sigma J_2\gamma_{2k}G_3+(E+6\sigma J_2)G_4=\frac{i}{2\pi}\left\langle\left[\hat{S}^-(a_4),\hat{B}\right]\right\rangle$$

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

$$E^4-2AE^2+B=0 \tag{25}$$

with

$$A=\sigma^2J_2^2(z_2^2-\gamma_{2k}^2),\ B=\sigma^4\left[J_2^4(z_2^2-\gamma_{2k}^2)^2-J_1^4(\gamma_{1k}^2-\gamma_{1k}^{*2})^2-4J_1^2J_2^2\,|\,6\gamma_{1k}-\gamma_{1k}^*\gamma_{2k}\,|^2\right],z_1=4,z_2=6 \tag{26}$$

giving four magnon branches

$$E_{1,2k}=\pm\sqrt{A-\sqrt{A^2-B}},\ E_{3,4k}=\pm\sqrt{A+\sqrt{A^2-B}}.\tag{27}$$

These can be also written as

$$E_{1k}=\sigma J_1\sqrt{\left(\frac{J_2}{J_1}\right)^2(z_2^2-\gamma_{2k}^2)+K},\ E_{3k}=\sigma J_1\sqrt{\left(\frac{J_2}{J_1}\right)^2(z_2^2-\gamma_{2k}^2)-K}, \tag{28}$$

$$(E_{2k}=-E_{1k},\ E_{4k}=-E_{3k}),\quad K=\sqrt{(\gamma_{1k}^2-\gamma_{1k}^{*2})^2+4\left(\frac{J_2}{J_1}\right)|\,6\gamma_{1k}-\gamma_{1k}^*\gamma_{2k}\,|^2}$$

Choosing Green's functions for convenient operators, we can calculate the sublattice magnetization in AF2 phase

$$\sigma=\left\{\frac{J_2}{J_1}\frac{1}{N}\sum_k\frac{1}{K}\left[\frac{6K+12\,|\,\gamma_{1k}\,|^2-\gamma_{2k}(\gamma_{1k}^2+\gamma_{1k}^{*2})}{\sqrt{\left(\frac{J_2}{J_1}\right)^2(z_2^2-\gamma_{2k}^2)+K}}\coth\frac{E_{1k}}{2T}+\frac{6K-12\,|\,\gamma_{1k}\,|^2+\gamma_{2k}(\gamma_{1k}^2+\gamma_{1k}^{*2})}{\sqrt{\left(\frac{J_2}{J_1}\right)^2(z_2^2-\gamma_{2k}^2)-K}}\coth\frac{E_{3k}}{2T}\right]\right\}^{-1} \tag{29}$$

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

$$\begin{aligned}\frac{\left\langle\hat{H}_{AF2}\right\rangle}{J_1N}=\frac{\sigma_0}{4N}\sum_k\Bigg[&\frac{-2K\,|\,\gamma_{1k}\,|^2+\left(\gamma_{1k}^2-\gamma_{1k}^{*2}\right)^2-12p^2\left(\gamma_{1k}^2+\gamma_{1k}^{*2}\right)\gamma_{2k}+4p^2\,|\,\gamma_{1k}\,|^2\,\gamma_{2k}^2}{K\cdot K_1}\\
&+\frac{-2K\,|\,\gamma_{1k}\,|^2-\left(\gamma_{1k}^2-\gamma_{1k}^{*2}\right)^2+12p^2\left(\gamma_{1k}^2+\gamma_{1k}^{*2}\right)\gamma_{2k}-4p^2\,|\,\gamma_{1k}\,|^2\,\gamma_{2k}^2}{K\cdot K_3}\\
&+\frac{\left(\gamma_{1k}^2-\gamma_{1k}^{*2}\right)^2+2\,|\,\gamma_{1k}\,|^2\left(K+72p^2\right)-12p^2\left(\gamma_{1k}^2+\gamma_{1k}^{*2}\right)\gamma_{2k}}{K\cdot K_1}\\
&+\frac{-\left(\gamma_{1k}^2-\gamma_{1k}^{*2}\right)^2+2\,|\,\gamma_{1k}\,|^2\left(K-72p^2\right)+12p^2\left(\gamma_{1k}^2+\gamma_{1k}^{*2}\right)\gamma_{2k}}{K\cdot K_3}\Bigg]\\
&+\frac{\sigma_0}{2N}\sum_k\frac{p^2\gamma_{2k}}{K}\left[\frac{2\,|\,\gamma_{1k}\,|^2\,\gamma_{2k}-6\left(\gamma_{1k}^2+\gamma_{1k}^{*2}\right)-\gamma_{2k}K}{K_1}+\frac{-2\,|\,\gamma_{1k}\,|^2\,\gamma_{2k}+6\left(\gamma_{1k}^2+\gamma_{1k}^{*2}\right)-\gamma_{2k}K}{K_3}\right]\end{aligned}$$

$$+\frac{\sigma_0^2}{N}\sum_k\left[K_1+K_3-12p\right]-6p\sigma_0 \tag{30}$$

with σ_0 defined by (29) and $K_1=\sqrt{\left(\frac{J_2}{J_1}\right)^2(z_2^2-\gamma_{2k}^2)+K}$, $K_3=\sqrt{\left(\frac{J_2}{J_1}\right)^2(z_2^2-\gamma_{2k}^2)-K}$ and $p=J_2/J_1$.

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 $p=J_2/J_1\approx 0.65$. 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.

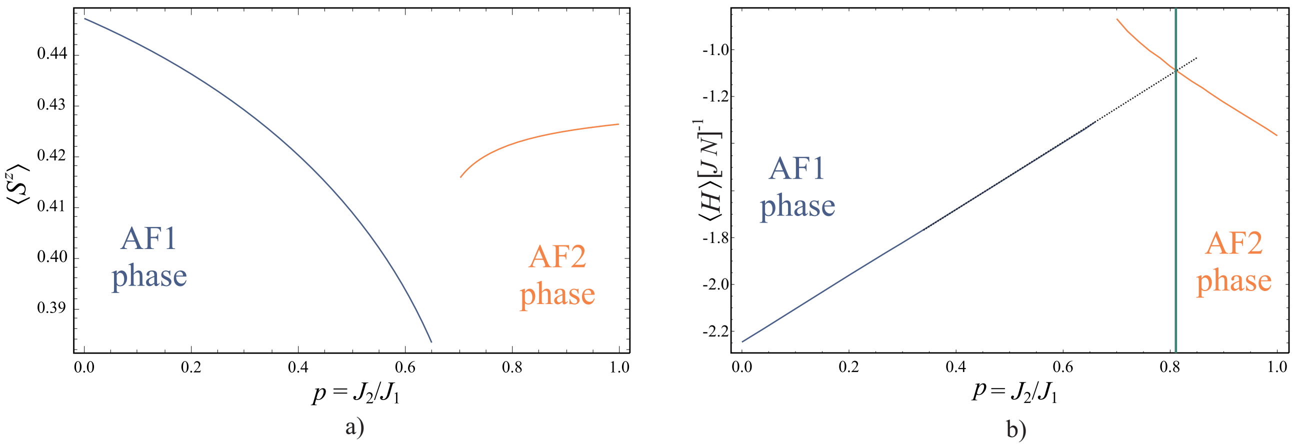

Figure 2. a) Ground state magnetization and b) internal energy of frustrated spin ½ Heisenberg antiferromagnet on bcc lattice. Dashed line (for p>0.65) denotes extrapolation.

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.

4. ACKNOWLEDGMENT

This work was supported by the Serbian Ministry of Education and Science: Grant No 171009.

5. REFERENCES

[1] T. H. Diep, *Frustrated Spin Systems*, 1st ed. World Scientific, Singapore 2004.

[2] X. G. Wen, *Quantum Field Theory of Many Body Systems*, Oxford University Press, 2007.

[3] S. Jin, A. Sen, A.W. Sandvik, *Ashkin-Teller Criticality and Pseudo-First-Order Behavior in a Frustrated Ising Model on the Square Lattice*, Phys. Rev. Lett., Vol. 108 (2012) 045702.

[4] G. R. Stewart, *Superconductivity in iron compounds*, Rev. Mod. Phys., Vol. 83 (2011) 1589−1652.

[5] D. C. Johnston, *The puzzle of high temperature superconductivity in layered iron pnictides and chalcogenides*, Adv. Phys., Vol. 59 (2010) 803−1061.

[6] J. S. Smart, *Effective Field Theories of Magnetism*, Saunders, Philadelphia 1966.

[7] J. Oitmaa and W. Zhang, *Phase diagram of the bcc* S-1/2 *Heisenberg antiferromagnet with first and second neighbor exchange*, Phys. Rev. B, Vol. 69 (2004) 064416.

[8] R. Schmidt, J. Schulenburg, J. Richter, and D.D. Betts, *Spin*-1/2 *model on the body-centered cubic lattice*, Phys. Rev. B, Vol. 66 (2002) 224406.

[9] K. Majumdar and T. Datta, *Non-linear spin wave theory results for the frustrated S-1/2 Heisenberg antiferromagnet on a body-centered cubic lattice*, J. Phys. Cond. Matt., Vol. 21 (2009) 046001.

[10] K. Majumdar, *Magnetic phase diagram of a spatially anisotropic, frustrated spin*-1/2 *Heisenberg antiferromagnet on a stacked square lattice*, J. Phys. Cond. Matt., Vol. 23 (2011) 406004.

[11] D. N. Zubarev, *Double-time Green functions in statistical physics*, Sov. Phys. Usp., Vol. 3 (1960) 320−342.

[12] S. V. Tyablikov, *The Methods in the Quantum Theory of Magnetism*, Plenum Press, New York 1967.

[13] M. Manojlović, M. Pavkov-Hrvojević, M. Škrinjar, M. Pantić, D. Kapor, S. Stojanović, *Spin-wave dispersion and transition temperature in the cuprate antiferromagnet* La_2CuO_4, Phys. Rev. B, Vol. 68 (2003) 014435.

[14] S. Radošević, M. Pantić, M. Rutonjski, D. Kapor, M. Škrinjar, *Magnetic properties of quasi two-dimensional antiferromagnet* Rb_2MnCl_4 *with XXZ interaction anisotropy*, Eur. Phys. J. B, Vol. 68 (2009) 511−517.

[15] W. Nolting, A. Ramakanth, *Quantum Theory of Magnetism*, Springerr-Verlag, Berlin 2009.

[16] P. Frobrich, P.J. Kuntz, *Many-body Green's function theory of Heisenberg films*, Physics Reports, Vol. 432 (2006) 223−304.

[17] M. Rutonjski, S. Radošević, M. Škrinjar, M. Pavkov-Hrvojević, D. Kapor, M. Pantić, *Temperature dependence of sublattice magnetization in quasi-two-dimensional* S=1/2 *cuprate antiferromagnets: Green's function approach*, Phys. Rev. B, Vol. 76 (2007) 172506.

[18] S. Radošević, M. Rutonjski, M. Pantić, M. Pavkov-Hrvojević, D. Kapor, M. Škrinjar, *The Néel temperature of a D-dimensional bcc Heisenberg antiferromagnet*, Solid State Commun., Vol. 151 (2011) 1753−1757.

[19] M. Rutonjski, S. Radošević, M. Pantić, M. Pavkov-Hrvojević, D. Kapor, M. Škrinjar, *Magnon specific heat of high*-T_c *parent compounds* La_2CuO_4 and $YBa_2Cu_3O_6$: *Green's function approach*, Solid State Commun., Vol. 151 (2011) 518−522.

[20] M. R. Pantić, D. V. Kapor, S. M. Radošević, and P. M. Mali, *Phase diagram of quantum Heisenberg* J_1–J_2 *antiferromagnet on the body-centered-cubic lattice in random phase approximation*, Solid State Commun., Vol. 182 (2014) 55−58.

УНУТРАШЊА ЕНЕРГИЈА ХАЈЗЕНБЕРГОВОГ J_1-J_2 АНТИФЕРОМАГНЕТА СА СПИНОМ 1/2 НА ЗАПРЕМИНСКИ ЦЕНТРИРАНОЈ КУБНОЈ РЕШЕТКИ У АПРОКСИМАЦИЈИ ТЈАБЛИКОВА

Сажетак: У раду су истражена магнетна својства квантног Хајзенберговог J_1-J_2 антиферомагнета са спином 1/2 на запремински центрираној кубној решетки. Користећи метод двовременских температурских Гринових функција, добијена је зависност магнетизације подрешетке и критичне температуре од параметра фрустрације J_2/J_1 како у колинеарној, тако и у Неловој фази. Анализа магнетизације подрешетке у основном стању, као и унутрашње енергије, указују на фазни прелаз првог реда из Нелове у колинеарну фазу за $0.7 < J_2/J_1 < 0.8$, што је у складу са ранијим истраживањима.

Кључне речи: Хајзенбергов J_1-J_2 антиферомагнет, унутрашња енергија, Нелова и колинеарна фаза, апроксимација Тјабликова.