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ANISOTROPY INFLUENCE ON THE STRIPED ANTIFERROMAGNETISM OF A FRUSTRATED HEISENBERG MODEL: AN APPLICATION TO IRON PNICTIDE MATERIALS

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Abstract: Motivated by several experimental studies of magnetic compounds related to iron pnictides, we examine thermodynamic properties of anisotropic J_{1a} - J_{1b} - J_c - J_2 Heisenberg antiferromagnetic model. Our calculations are based on the two-time temperature Green's functions within several well-known decoupling approximations. We obtain excitation spectrum, correlation functions and the analytic expression for the critical temperature and compare our results to the existing experimental data. Results presented here could be of a great importance in the further investigations of similar magnetic systems.

Keywords: Frustrated Heisenberg J_{1a} - J_{1b} - J_c - J_2 antiferromagnet, iron pnictides, spin anisotropy, spin stripe phase, neel temperature.

1. INTRODUCTION

Recent synthesis [1] of the new class of high-T_C superconductors, namely the iron-based layered compounds [1-10], for instance the compounds of the ReOFeAs type (Re denotes rare earth elements: La, Ce, Pr, Nd, Sm,...), also known as 1111-systems, or the so-called 122-systems like AFe_2As_2 (A= Ba, Sr, Ca) etc., aroused great interest in the investigation of these materials. In the undoped regime, these compounds are usually metals ordered antiferromagnetically [10] below the Neel temperature T_N (for LaOFeAs $T_N \cong 137K$), while upon doping they become superconducting with the long-range order destroyed. The common structure elements of these compounds are the conducting FeAS layers, wherefore they are known as the ferropnictides. Since the discovery of the antiferromagnetic (AFM) long-range order in these high-T_C superconducting parent compounds, the correlation between their magnetic and superconducting properties has been examined. Namely, the superconductivity and magnetism are competitive phenomena. Shortly after the discovery of the 1111-type compounds, followed the discovery of the 122-type compounds which contain the double FeAs layers within the unit cell. This affected the primacy of the cuprates in the high-T_C superconductor physics, leading to the progress in the synthesis of the new high-T_C superconductors and encouraging further theoretical studies devoted to understanding of the mechanism of high-T_C superconductivity.

The analogy between ferropnictides and cuprates becomes more profound when their crystal structures are compared. Namely, FeAs systems of 1111-type consist of the FeAs planes separated by the ReO layers, similar to the cuprates where CuO_2 planes are separated by LaBa or YBa layers. Within the FeAs plane, every Fe atom is surrounded by As atoms. It should be emphasized that FeAs planes in fact present the triple sandwich with the quadratic lattice of Fe atoms in the middle and quadratic lattices of As atoms above and below whereby the latest two are shifted in the way that every Fe atom is surrounded by the tetrahedron of As atoms. Due to the complex structure, both ferropnictides and cuprates are highly anisotropic, yielding the strong anisotropy of the superconducting and magnetic properties, as well their pronounced quasi-two-dimensionality. The crystal structure of LaOFeAs is presented in Figure 1a. The unit cell is tetragonal with the following parameters: $a = b = 4.035 \cdot 10^{-10} m$, $c = 8.740 \cdot 10^{-10} m$. The parameters characterizing other compounds of the 1111-type are very close to the mentioned ones. Obviously, the tetragonality of the unit cell (a=b<c) stipulates the quasi-2D character of these compounds.

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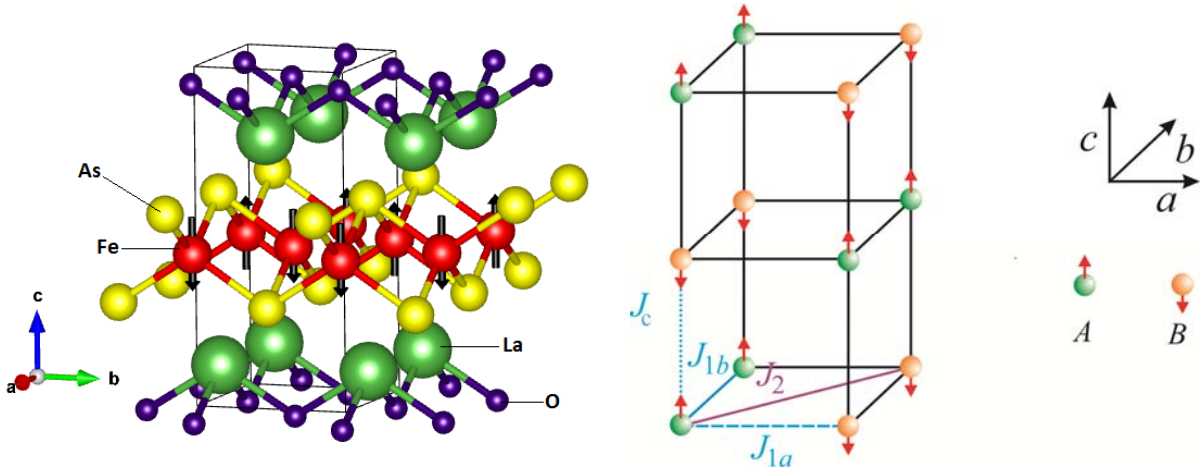

Figure1. a) Crystal structure of LaOFeAs in undoped regime, b) Magnetic unit cell of this compound with the dominant spin interactions labeled

Detailed calculations have shown that the AFM phase is for LaOFeAs more stable than the non-magnetic state [11,12], whereby the AFM ground state has a special [2,10] type of order – stripe-like order within the *ab* plane where the spins in one column are predominantly oriented in one direction (Figure 2), which is due to the AFM coupling further repeated along the *c* direction, as shown in Figure 1b. The corresponding exchange interactions are denoted in the same Figure.

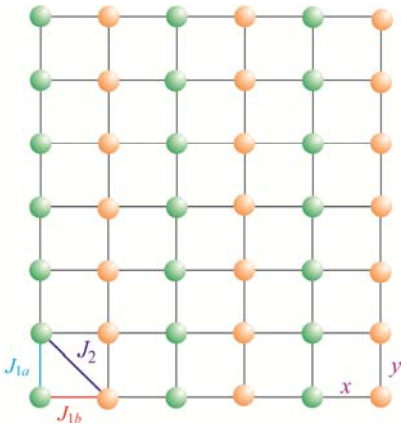

Figure 2. Striped spin order. Green and yellow circles denote the spins oriented in opposite directions

The magnetic properties in these compounds are due to Fe^{2+} ions, which form the magnetic unit cell (Figure 1b). In this case, magnetism results from the spins of the unpaired electrons in the 3d shell of the iron ion. Band theory predicts that there can exist at most two unpaired electrons per Fe site [13,14]. Layers which separate the FeAs planes do not exhibit magnetism, which induces the quasi-2D character of the magnetic lattice. Regarding the ReOFeAs-type compounds in the undoped regime, they possess AFM order with the magnetic phase transitions at $T<T_N=150K$. As it is already mentioned, upon either hole or electron doping, the long-range magnetic order in FeAs systems vanishes and superconductive phase emerges, the fact confirmed by the neutron scattering experiments [15,16], muon spin resonance and Mossbauer spectroscopy [17,18].

Therefore, similarly to the cuprates, the superconductivity in the ferropnictides occurs close to the magnetic phase transition, which may suggest that the AFM fluctuations play an important role in the electron coupling. Magnetic order, i.e. the transition from the paramagnetic to AFM phase in ferropnicitides appears in the temperature interval from 100 to 200 K [19]. For instance, the compound LaOFeAS which is the subject of our analysis becomes antiferromagnetically ordered at $T_N=137K$ [10]. In the 122-systems like AFe_2As_2, magnetic phase transition occurs at the temperature equal or slightly lower than the temperature of the tetragonal-to-orthorhombic structural phase transition. The fact that the magnetic and structural phase transition occur at almost the same temperature suggests that these two transitions are correlated. In this paper, we neglect the structural phase transition and assume that the crystal structure of the 1111-type of the ferropnictides is tetragonal in the whole temperature range below T_N.

The substitution of oxygen atoms in ReOFeAS-type compounds by fluorine or some other rare earth element, leads to the rapid decrease of Neel temperature [2,8,10], whereby for the critical value of the dopant concentration ($x_c \approx 0.1$) long-range magnetic order disappears, being replaced by the superconducting phase. It is interesting to observe that the magnetic properties of the 1111-type compounds are mainly determined by the characteristics of the single-ion magnetic anisotropy of the rare earth elements, as well as by the character of the interaction between two different magnetic systems:

subsystem formed by the localized 4f electrons of the rare earth and iron subsystem formed by the electrons in the 3d zone. This question, however, has not been clarified yet and requires a systematic research of the anisotropic properties of both systems. Regarding the theoretical models for the description of the magnon spectrum, two basic models are proposed [2]. Having in mind that the ReOFeAS-type compounds possess stripe-like AFM structure, the spin-wave spectrum and the Neel temperature are usually determined within the well-known AFM J_1-J_2 localized spin model [20,21] with its numerous modifications and different anisotropy types (single-ion, spin anisotropy, biquadratic interaction etc.) [10]. A possible and widely exploited modification of the model is effective 3D anisotropic Heisenberg AFM J_{1a}-J_{1b}-J_c-J_2 model, also used in this paper. The other model used in the study of the ferropnictides is the itinerant electron model for the 3d iron electrons [22,23]. The neutron scattering experiments have shown that the J_1-J_2 model describes satisfactorily the low energy part of the magnon spectrum, below 100 meV [24-26], while the itinerant electron model describes the spin excitations at higher energies [26].

Besides, these compounds present the systems with the spin frustration. Frustrated magnetic systems have been intensively studied both theoretically and experimentally over the last decades [27,28]. It was shown that the collinear or stripe-like structure can be described by the Heisenberg model with the nearest and the next-nearest neighbour interactions. Magnetic phases and the AFM properties of the ferropnictides with the different exchange interactions taken into account have also been studied within the other theoretical approaches, for instance spin-wave theory, GF method etc. [29−35]. Aforementioned papers and different methods used therein may be useful for the understanding of the mechanism of superconductivity in the iron-based superconductors.

In this paper, we do not examine the origin and the nature of different magnetic anisotropy types in the 1111-systems. We instead calculate the spin-wave spectrum, and based upon that expression we determine Neel temperature as well as the spin-gap within the framework of the effective 3D anisotropic HAF J_{1a}-J_{1b}-J_c-J_2 model containing NN and NNN exchange interactions labeled by $J_{1/2}$. Thereby, we assume that the interplanar exchange interaction J_c is much smaller than the NN interaction within the *ab* plane, $J_c << J_{1a,b}$. We also examine the influence of the interplanar interaction J_c on certain thermodynamic properties of 1111-systems. Similar model, as well as the corresponding RPA, was used in the analysis of the magnetic properties of the cuprates in the undoped regime [36−44].

The main idea of this paper is to choose the specific anisotropy in the model spin Hamiltonian, based upon the model parameters known from literature. We restrict ourselves to the spin magnetic anisotropy and derive the expression for the Neel temperature in dependence of the exchange integrals and the spin anisotropy parameter. Having at our disposal the experimental data for the exchange integrals and the Neel temperature, we determine the spin anisotropy parameter to reproduce the experimental value of T_N. We use the two-time temperature Green function (GF) method for the Heisenberg model with arbitrary spin (specially for LaOFeAs S=1), by making use of the Tyablikov self-consistent approach [45] and the well-known random phase approximation (RPA). We also compare the obtained results to the ones following from the LSW approach. That is, we use the Green functions for both the spin and boson operators in order to determine the relevant thermodynamic properties of the LaOFeAs system.

The paper is organized as follows: After a descriptive introduction, in Section 2 we formulate the anisotropic model and derive analytically main results within the aforementioned approximations by making use of the GF method. In Sec. 3, we perform the bosonization and give some basic results of the LSW theory. The following Section is devoted to the numerical calculations, comparison to the experimental results and discussion of the obtained results. Finally, we summarize the conclusions and quote the references.

2. MODEL HAMILTONIAN. GREEN'S FUNCTION DETERMINATION AND MAIN RESULTS

In order to describe the striped antiferromagnetic long-range order of the LaOFeAs structure, we have to take into account the intra- and interplanar NN interactions, as well as the NNN interactions within the *ab*-planes. As an initial point, we take the following J_1-J_2 quantum Heisenberg model

$$\hat{H} = J_1 \sum_{\langle i,j;\alpha,\beta\rangle} \vec{S}_i(\alpha)\cdot\vec{S}_j(\beta) + J_2 \sum_{\langle\langle i,j;\alpha,\beta\rangle\rangle} \vec{S}_i(\alpha)\cdot\vec{S}_j(\beta) \quad (1)$$

where $\langle i,j\rangle$ denotes the nearest-neighbour spin pairs, $\langle\langle i,j\rangle\rangle$ stands for the next-nearest-neighbours, while two sublattices in the magnetic unit cell are denoted by α,β. The position vectors of the magnetic lattice sites will be italicized (i,j) (instead of bold) throughout the paper, bearing in mind that we deal with the vectors. The exchange integrals in Eq. (1) are assumed to be antiferromagnetic, i.e. $J_1, J_2 > 0$. The ferro-

magnetic NN interaction ($J_1<0$) in the Hamiltonian of type (1) was analyzed in [21,29]. At this point, we should emphasize an important difference between FM and AFM materials. Namely, in the ground state of the ferromagnets, all spins are directed in the same way, wherefore the relative magnetization of the system at T=0K is for arbitrary spin S maximal and equals S. Only with the increase of temperature, thermal fluctuations occur, leading to the reduction of the relative magnetization. The antiferromagnetic crystalline system consists, however, of two or more interpenetrating equivalent magnetic sublattices, whereby the neighbouring spins point in different directions – the so-called Neel state. Even at T=0K, in the antiferromagnetic systems quantum fluctuations occur, yielding the reduction of the net magnetization. Therefore, if we kept only the NN terms in Hamiltonian (1), the ground state would not be exactly the Neel state, due to the quantum fluctuations [46]. The examinations based on the comprehensive Hamiltonian of type (1) (see [21,32-35]) have shown that the ground state of the system depends on the exchange integral ratio $p = J_2 / J_1$, referred to as the frustration parameter. Generally, it is considered that the stripe-like magnetic order can exist for the frustration parameter $p = J_2 / J_1 > 0.5$. Reducing the ratio J_2 / J_1 to some critical value, the stripe-like order becomes unstable and gets replaced by a ground state without the long-range magnetic order [47]. Quantum fluctuations occur also in the stripe-like phase, leading to the magnetization reduction in the whole temperature range in which this phase exists. In this paper, we are interested in the three-dimensional generalization of the J_1-J_2 model. That is, beside the intraplanar NN and NNN interactions, we take into account much weaker interplanar interactions, characterized by the exchange integral J_c. This implies the J_1-J_2-J_c model described by the following Hamiltonian:

$$\hat{H} = J_1 \sum_{\langle i,j;\alpha,\beta\rangle} \vec{S}_i(\alpha)\cdot\vec{S}_j(\beta) + J_2 \sum_{\langle\langle i,j;\alpha,\beta\rangle\rangle} \vec{S}_i(\alpha)\cdot\vec{S}_j(\beta) + J_c \sum_{|i,j;\alpha,\beta|} \vec{S}_i(\alpha)\cdot\vec{S}_j(\beta) \tag{2}$$

where $|i,j;\alpha,\beta|$ denotes the NN spin pairs, belonging to the adjacent planes. Due to the aforementioned layered structure and much bigger lattice constant in the crystallographic axis *c*, the exchange integral J_c is at least ten times smaller than J_1, J_2. Let us also remember that in the type 1111 of the ferropnictides, we shall neglect the structural phase transition and assume that the crystallographic unit cell is tetragonal. The magnetic unit cell of the type-1111 structure is presented schematically in Figure 1b, whereby the spins are associated with the magnetic ions Fe^{2+}. The magnetic unit cell volume for LaOFeAs equals $V_0=a^2c$, while the lattice constants read: $a = b = 4.035\cdot10^{-10} m,\ c = 8.740\cdot10^{-10} m$. The tetragonality of the magnetic lattice is taken into account through different exchange integrals J_1 and J_c. However, in order to determine the relevant thermodynamic properties of the compound LaOFeAs, in this paper we shall study the generalized spin-1 anisotropic Heisenberg AFM J_{1a}-J_{1b}-J_c-J_2 model. As regards the system parameter values, for now they are restricted only by the fact that they should allow the existence of the stripe-like AFM phase. Finally, from Figure 1b it is obvious that the system has two sublattices, A and B, with the antiparallel spin orientation.

Let us now go back to the model Hamiltonian (2), i.e. its modified version J_{1a}-J_{1b}-J_c-J_2. First, we have to replace the operators $\hat{S}_i^x(\alpha), \hat{S}_i^y(\alpha), \hat{S}_i^z(\alpha)$ by the spin raising and lowering operators:

$$\hat{S}_i^+(\alpha) = \hat{S}_i^x(\alpha) + i\,\hat{S}_i^y(\alpha), \quad \hat{S}_i^-(\alpha) = \hat{S}_i^x(\alpha) - i\,\hat{S}_i^y(\alpha) \tag{2a}$$

These operators $\hat{S}_i^-(\alpha)$ i $\hat{S}_i^+(\alpha)$ directly correspond to the physical picture of the processional motion of the individual spins, whereby their *z*-projections get either raised or lowered. The operator $\hat{S}_i^-(\alpha)$ creates the excitations in the sublattice $\alpha = A, B$ (lowers the *z*-projection of the spin at the site *i* within the sublattice), while the operator $\hat{S}_i^+(\alpha)$ annihilates them (raises the *z*-projection of the spin). The commutation relations for the operators $\hat{S}_i^+(\alpha), \hat{S}_i^-(\alpha), \hat{S}_i^z(\alpha)$ read [45]:

$$\left[\hat{S}_i^+(\alpha), \hat{S}_j^-(\beta)\right] = 2\hat{S}_i^z(\alpha)\delta_{ij}\,\delta_{\alpha\beta}, \quad \left[\hat{S}_i^\pm(\alpha), \hat{S}_j^z(\beta)\right] = \mp\hat{S}_i^\pm(\alpha)\delta_{ij}\,\delta_{\alpha\beta} \tag{2b}$$

Besides, one should bear in mind additional relations:

$$\left(\vec{S}_i(\alpha)\cdot\vec{S}_i(\alpha)\right) = \left(\hat{S}_i^x(\alpha)\right)^2 + \left(\hat{S}_i^y(\alpha)\right)^2 + \left(\hat{S}_i^z(\alpha)\right)^2 = S(S+1) \tag{2c}$$

$$\prod_{p=-S}^{S}\left(\hat{S}_i^z(\alpha) - p\right) = 0, \tag{2d}$$

$$\left(\hat{S}_i^+(\alpha)\right)^{2S+1} = \left(\hat{S}_i^-(\alpha)\right)^{2S+1} = 0 \tag{2e}$$

The relation (2d) shows that the *z*-projection of the spin may take only finite values ranging from –S to S in steps of one. Therefore the spin space is finite-dimensional with the dimension 2S+1, where S denotes the spin quantum number which characterizes the system. The allowed values for S are integers and half-integers. Since the spin *z*-projection is limited to the interval from $-S$ to S, the operators $\hat{S}_i^-(\alpha)$ i $\hat{S}_i^+(\alpha)$ can create/annihilate at most $2S$ excitations at the given lattice site, which is expressed by the relation (2e).

Since LaOFeAs is antiferromagnetically ordered, in order to determine the spin-wave spectrum, we first introduce the local coordinate system on the sublattice B. This is achieved through the unitary transformation of the spin operators on each site of the sublattice B [48], i.e. performing in the spin space the rotation around *x*-axis by π. Thus the spin operators $\hat{S}_j^{\nu}$ become:

$$\begin{aligned}
&\hat{S}_j^{'x} = \hat{S}_j^x, \quad \hat{S}_j^{'y} = -\hat{S}_j^y, \quad \hat{S}_j^{'z} = -\hat{S}_j^z, \\
&\hat{S}_j^{'+} = \hat{S}_j^{'x} + iS_j^{'y} = \hat{S}_j^x - i\hat{S}_j^y = \hat{S}_j^-, \\
&\hat{S}_j^{'-} = \hat{S}_j^{'x} - iS_j^{'y} = \hat{S}_j^x + i\hat{S}_j^y = \hat{S}_j^+
\end{aligned} \tag{3}$$

In this new coordinate system all magnetic moments (spins) are oriented in the same direction $\hat{S}_j^{'z}$ with the unique quantization axis, which significantly simplifies further calculations and theoretical analysis. It is obvious that due to the unitary transformation (3) the Neel state formally looks like the ferromagnetic ground state.

After performing the unitary transformation (3), we can rewrite the Hamiltonian in the local coordinate system as follows:

$$\begin{aligned}
\hat{H} = {} & J_{1a}\sum_{i,\lambda_1^x}\left(\vec{S}_i(A)\cdot\vec{S}_{i+\lambda_1^x}(B) - \delta\hat{S}_i^z(A)\hat{S}_{i+\lambda_1^x}^z(B)\right) + \frac{J_{1b}}{2}\sum_{i,\lambda_1^y}\left(\vec{S}_i(A)\cdot\vec{S}_{i+\lambda_1^y}(A) + \delta\hat{S}_i^z(A)\hat{S}_{i+\lambda_1^y}^z(A)\right) + \\
& + (A\to B) + J_c\sum_{i,\lambda_1^z}\left(\vec{S}_i(A)\cdot\vec{S}_{i+\lambda_1^z}(B) - \delta\hat{S}_i^z(A)\hat{S}_{i+\lambda_1^z}^z(B)\right) + J_2\sum_{i,\lambda_2}\vec{S}_i(A)\cdot\vec{S}_{i+\lambda_2}(B)
\end{aligned} \tag{4}$$

where $\hat{S}_i(A)$ denotes the quantum spin operator at site *i* of either sublattice, $\lambda_1^x, \lambda_1^y, \lambda_1^z$ signify the distances to the NN in corresponding directions, λ_2 refers to the NNN within the *ab* plane, while $\eta = 1+\delta, \delta \geq 0$ presents the spin anisotropy parameter. While the numerical values of the exchange integrals can be found in earlier papers, both theoretical and experimental [49,50], the parameter $\delta \geq 0$ will be determined theoretically within our approach. Let us note that due to the collinear phase, $J_2 > J_{1a}/2$, $J_{1b}/2$. Besides, all exchange integrals in this model are positive, i.e. all interactions are assumed to be antiferromagnetic. The ferromagnetic J_1 was analyzed in our paper [29]. Making use of the Eqs. (2a-e), we can replace the parameters $\hat{S}_i^{x/y}(\alpha)$ in Hamiltonian (4) by the operators $\hat{S}_i^{-/+}(\alpha)$ as follows:

$$\vec{S}_i(\alpha)\cdot\vec{S}_j(\beta) = \frac{1}{2}\left(\hat{S}_i^+(\alpha)\hat{S}_j^-(\beta) + \hat{S}_i^-(\alpha)\hat{S}_j^+(\beta)\right) + \hat{S}_i^z(\alpha)\hat{S}_i^z(\beta) \tag{4a}$$

After the aforementioned rotation in the spin space is performed, the terms of the type $\vec{S}_i(\alpha)\cdot\vec{S}_j(\beta)$ become

$$\vec{S}_i(\alpha)\cdot\vec{S}_j(\beta) = \frac{1}{2}\left(\hat{S}_i^+(\alpha)\hat{S}_j^+(\beta) + \hat{S}_i^-(\alpha)\hat{S}_j^-(\beta)\right) - \hat{S}_i^z(\alpha)\hat{S}_i^z(\beta) \tag{4b}$$

Using Eqs. (4a) and (4b), the Hamiltonian in the local coordinate system rewritten in terms of the operators $\hat{S}_i^+(\alpha), \hat{S}_i^-(\alpha)$ and $\hat{S}_i^z(\alpha)$, reads:

$$\begin{aligned}
\hat{H} = {} & J_{1a}\sum_{i,\lambda_1^x}\left(\frac{1}{2}\left(\hat{S}_i^-(A)\hat{S}_{i+\lambda_1^x}^-(B) + h.c.\right) - \eta\hat{S}_i^z(A)\hat{S}_{i+\lambda_1^x}^z(B)\right) + \\
& + \frac{J_{1b}}{2}\sum_{i,\lambda_1^y}\left(\frac{1}{2}\left(\hat{S}_i^-(A)\hat{S}_{i+\lambda_1^y}^+(A) + h.c.\right) + \eta\hat{S}_i^z(A)\hat{S}_{i+\lambda_1^y}^z(A)\right) + (A\to B) + \\
& + J_c\sum_{i,\lambda_1^z}\left(\frac{1}{2}\left(\hat{S}_i^-(A)\hat{S}_{i+\lambda_1^z}^-(B) + h.c.\right) - \eta\hat{S}_i^z(A)\hat{S}_{i+\lambda_1^z}^z(B)\right) + \\
& + J_2\sum_{i,\lambda_2}\left(\frac{1}{2}\left(\hat{S}_i^-(A)\hat{S}_{i+\lambda_2}^-(B) + h.c.\right) - \hat{S}_i^z(A)\hat{S}_{i+\lambda_2}^z(B)\right),
\end{aligned} \tag{4c}$$

where the notation is consistent with that used in Figs. 1 and 2. Throughout the paper "h.c." denotes "hermitian conjugate" and we have set $\hbar = 1$.

We first perform the calculations within the spin Green`s function method. Therefore, we analyze the system for arbitrary spin S, specially

S=1 for LaOFeAS, using the formalism of two-time temperature dependent Green's functions (GF) [45], since within that method all relevant thermodynamic system properties can be obtained self-consistently. For an application of GFs technique on Heisenberg AFMs, please see the references [51-57]. Retarded two-time GF [45] is defined as follows:

$$G_{n,m}(t,t') = \left\langle\left\langle \hat{A}_n(t) \,|\hat{Q}_m(t')\right\rangle\right\rangle = \theta(t-t')\left\langle[\hat{A}_n(t),\hat{Q}_m(t')]\right\rangle \quad (5)$$

where $\theta(t-t')$ denotes the Heaviside step function, defined as $\theta(t-t')=1, \quad t>t'$, while $\theta(t-t')=0, \quad t<t'$. The quantity $[\hat{A},\hat{B}]=\hat{A}\hat{B}-\hat{B}\hat{A}$, $\hat{A}(t)=e^{i\hat{H}t}\hat{A}e^{-i\hat{H}t}$ presents the commutator of the operators $\hat{A}$ and $\hat{B}$ in the Heisenberg picture, while $\left\langle \hat{A}\hat{B}\right\rangle$ presents the ensemble average at temperature T calculated with the Hamiltonian (4). In our case operators $\hat{A}$ and $\hat{Q}$ will be the spin (or boson) operators located at particular site $n(m)$ belonging to the sublattice $\alpha = A,B$: $S_n^i(\alpha)(i=+,-)$. 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 so called Tyablikov's decoupling or Random Phase Approximation (RPA) in the following manner:

$$\left\langle\left\langle \hat{S}_n^z(\alpha)\hat{S}_l^i(\beta)\,|\hat{Q}_m(\gamma)\right\rangle\right\rangle \cong \left\langle \hat{S}_n^z(\alpha)\right\rangle\left\langle\left\langle \hat{S}_l^i(\beta)\,|\hat{Q}_m(\gamma)\right\rangle\right\rangle \quad (6)$$

where $\hat{S}^+$ and $\hat{S}^-$ are standard spin rising and lowering operators and operator $\hat{Q}_m$ will be chosen in a convenient way latter (see [38,52] 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. Hence, we shall first close the system of equations for the GFs, by decoupling the higher-order GFs using (6). Afterwards, we shall perform the spatial and temporal Fourier-transform in the following manner:

$$\left\langle\left\langle \hat{S}_n^i(\alpha)\,|\hat{Q}_m(\beta)\right\rangle\right\rangle_{k,\omega} = \frac{1}{N}\sum_k e^{ik(n-m)}\int d(t-t')e^{i\omega(t-t')}\left\langle\left\langle \hat{S}_n^i(\alpha,t)\,|\hat{Q}_m(\beta,t')\right\rangle\right\rangle \quad . \quad (7)$$

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

In order to calculate the spin-wave spectrum in the model (4c), we use the method of equations of motions for the operators $\hat{S}_n^+(A), \hat{S}_n^-(B)$, i.e. $i\dfrac{d\hat{S}_n^+(A)}{dt} = i\hat{\dot{S}}_n^+(A) = [\hat{S}_n^+(A),\hat{H}]$ and the analogous equation $i\hat{\dot{S}}_n^-(b) = -\left([\hat{S}_n^-(B),\hat{H}]\right)^+$.

After having found the necessary commutators with the Hamiltonian (4c), we obtain the following system of equations:

$$i\frac{d\hat{S}_n^+(A)}{dt} = J_{1a}\sum_{\lambda_1^x}\left(\hat{S}_n^z(A)\hat{S}_{n+\lambda_1^x}^-(B)+\eta\,\hat{S}_n^+(A)\hat{S}_{n+\lambda_1^x}^z(B)\right)+J_{1b}\sum_{\lambda_1^y}\left(\hat{S}_n^z(A)\hat{S}_{n+\lambda_1^y}^+(A)-\eta\,\hat{S}_n^+(A)\hat{S}_{n+\lambda_1^y}^z(A)\right)+$$
$$+J_c\sum_{\lambda_1^z}\left(\hat{S}_n^z(A)\hat{S}_{n+\lambda_1^z}^-(B)+\eta\,\hat{S}_n^+(A)\hat{S}_{n+\lambda_1^z}^z(B)\right) \quad (8a)$$

$$i\frac{d\hat{S}_n^-(B)}{dt} = -J_{1a}\sum_{\lambda_1^x}\left(\hat{S}_n^z(B)\hat{S}_{n+\lambda_1^x}^+(A)+\eta\,\hat{S}_n^-(B)\hat{S}_{n+\lambda_1^x}^z(A)\right)-J_{1b}\sum_{\lambda_1^y}\left(\hat{S}_n^z(B)\hat{S}_{n+\lambda_1^y}^-(B)-\eta\,\hat{S}_n^-(B)\hat{S}_{n+\lambda_1^y}^z(B)\right)-$$
$$-J_c\sum_{\lambda_1^z}\left(\hat{S}_n^z(B)\hat{S}_{n+\lambda_1^z}^+(A)+\eta\,\hat{S}_n^-(B)\hat{S}_{n+\lambda_1^z}^z(A)\right)-J_2\sum_{\lambda_2}\left(\hat{S}_n^z(B)\hat{S}_{n+\lambda_2}^+(A)+\hat{S}_n^-(B)\hat{S}_{n+\lambda_2}^z(A)\right) \quad (8b)$$

Equations (8a,b) enable us to find easily the system of equations for GFs, where, as we have already mentioned, the operator $\hat{Q}_m$ presents a conveniently chosen spin operator. Finally, after the time-frequency Fourier transform

$$\left\langle\left\langle \hat{S}_n^i(\alpha,t)\,|\hat{Q}_m(\beta,t')\right\rangle\right\rangle = \int_{-\infty}^{+\infty} d\omega\, e^{-i\omega(t-t')}\left\langle\left\langle \hat{S}_n^i(\alpha)\,|\hat{Q}_m(\beta)\right\rangle\right\rangle_\omega \quad (9)$$

we obtain the following system of equations:

$$E\left\langle\left\langle \hat{S}_n^+(A)\,|\,\hat{Q}_m\right\rangle\right\rangle_\omega = \frac{i}{2\pi}\left\langle[\hat{S}_n^+(A),\hat{Q}_m]\right\rangle + J_{1a}\sum_{\lambda_1^x}\left(\left\langle\left\langle \hat{S}_n^z(A)\hat{S}^-_{n+\lambda_1^x}(B)\,|\,\hat{Q}_m\right\rangle\right\rangle_\omega + \eta\left\langle\left\langle \hat{S}_n^+(A)\hat{S}^z_{n+\lambda_1^x}(B)\,|\,\hat{Q}_m\right\rangle\right\rangle_\omega\right) +$$

$$+ J_{1b}\sum_{\lambda_1^y}\left(\left\langle\left\langle \hat{S}_n^z(A)\hat{S}^+_{n+\lambda_1^y}(A)\,|\,\hat{Q}_m\right\rangle\right\rangle_\omega - \eta\left\langle\left\langle \hat{S}_n^+(A)\hat{S}^z_{n+\lambda_1^y}(A)\,|\,\hat{Q}_m\right\rangle\right\rangle_\omega\right) + \tag{9a}$$

$$+ J_c\sum_{\lambda_1^z}\left(\left\langle\left\langle \hat{S}_n^z(A)\hat{S}^-_{n+\lambda_1^z}(B)\,|\,\hat{Q}_m\right\rangle\right\rangle_\omega + \eta\left\langle\left\langle \hat{S}_n^+(A)\hat{S}^z_{n+\lambda_1^z}(B)\,|\,\hat{Q}_m\right\rangle\right\rangle_\omega\right) +$$

$$+ J_2\sum_{\lambda_2}\left(\left\langle\left\langle \hat{S}_n^z(A)\hat{S}^-_{n+\lambda_2}(B)\,|\,\hat{Q}_m\right\rangle\right\rangle_\omega + \left\langle\left\langle \hat{S}_n^+(A)\hat{S}^z_{n+\lambda_2}(B)\,|\,\hat{Q}_m\right\rangle\right\rangle_\omega\right)$$

$$E\left\langle\left\langle \hat{S}_n^-(B)\,|\,\hat{Q}_m\right\rangle\right\rangle_\omega = \frac{i}{2\pi}\left\langle[\hat{S}_n^-(B),\hat{Q}_m]\right\rangle - J_{1a}\sum_{\lambda_1^x}\left(\left\langle\left\langle \hat{S}_n^z(B)\hat{S}^+_{n+\lambda_1^x}(A)\,|\,\hat{Q}_m\right\rangle\right\rangle_\omega + \eta\left\langle\left\langle \hat{S}_n^-(B)\hat{S}^z_{n+\lambda_1^x}(A)\,|\,\hat{Q}_m\right\rangle\right\rangle_\omega\right) -$$

$$- J_{1b}\sum_{\lambda_1^y}\left(\left\langle\left\langle \hat{S}_n^z(B)\hat{S}^-_{n+\lambda_1^y}(B)\,|\,\hat{Q}_m\right\rangle\right\rangle_\omega - \eta\left\langle\left\langle \hat{S}_n^-(B)\hat{S}^z_{n+\lambda_1^y}(B)\,|\,\hat{Q}_m\right\rangle\right\rangle_\omega\right) - \tag{9b}$$

$$- J_c\sum_{\lambda_1^z}\left(\left\langle\left\langle \hat{S}_n^z(B)\hat{S}^+_{n+\lambda_1^z}(A)\,|\,\hat{Q}_m\right\rangle\right\rangle_\omega + \eta\left\langle\left\langle \hat{S}_n^-(B)\hat{S}^z_{n+\lambda_1^z}(A)\,|\,\hat{Q}_m\right\rangle\right\rangle_\omega\right) -$$

$$- J_2\sum_{\lambda_2}\left(\left\langle\left\langle \hat{S}_n^z(B)\hat{S}^+_{n+\lambda_2}(A)\,|\,\hat{Q}_m\right\rangle\right\rangle_\omega + \left\langle\left\langle \hat{S}_n^-(B)\hat{S}^z_{n+\lambda_2}(A)\,|\,\hat{Q}_m\right\rangle\right\rangle_\omega\right)$$

Using Tyablikov RPA decoupling procedure (Eq. (6)), all higher-order GFs that appear on the right-hand side of Eqs. (9a,b) are expressed in terms of the lower-order ones. After performing the spatial Fourier transform

$$\left\langle\left\langle \hat{S}_n^i(\alpha)\,|\hat{Q}_m(\beta)\right\rangle\right\rangle_\omega = \frac{1}{N}\sum_k e^{ik(n-m)}\left\langle\left\langle \hat{S}^i(\alpha)\,|\hat{Q}(\beta)\right\rangle\right\rangle_{k,\omega}, \tag{9c}$$

we obtain the following closed system of equations for the GFs in (k,ω) - representation:

$$\left(E - A_k\right)\left\langle\left\langle \hat{S}^+(A)\,|\,\hat{Q}\right\rangle\right\rangle_{k,E} - B_k\left\langle\left\langle \hat{S}^-(B)\,|\,\hat{Q}\right\rangle\right\rangle_{k,E} = \frac{i}{2\pi}\left\langle\left[\hat{S}^+(A),\hat{Q}\right]\right\rangle_{k,E} \tag{10a}$$

$$B_k\left\langle\left\langle \hat{S}^+(a)\,|\,\hat{Q}\right\rangle\right\rangle_{k,E} + \left(E + A_k\right)\left\langle\left\langle \hat{S}^-(B)\,|\,\hat{Q}\right\rangle\right\rangle_{k,E} = \frac{i}{2\pi}\left\langle\left[\hat{S}^-(B),\hat{Q}\right]\right\rangle_{k,E} \tag{10b}$$

Here we use the following notation:

$$\begin{aligned} A_k &= 2\sigma\left[(J_{1a} - J_{1b} + J_c)\eta + J_{1b}\cos ak_y + 2J_2\right] = 2\sigma\, a(k) \\ B_k &= 2\sigma\left[J_{1a}\cos ak_x + J_c\cos ak_z + 2J_2\gamma_{2k}\right] = 2\sigma\, b(k) \end{aligned} \tag{11}$$

while the geometrical factor introduced in (11) read

$$\gamma_{2k} = \frac{1}{z_2}\sum_{\lambda_2} e^{ik\cdot\lambda_2} = \cos k_x a\,\cos k_y a\,, \tag{12}$$

where z_2 =4 denotes the number of the NNN within the plane.

Due to the rotation in the spin space, we assume that $\sigma(A) = \sigma(B) = \sigma$. This equality can be rigorously proved.

Vanishing determinant of the system (10a,b) gives the Green's functions poles, whereby the positive one which defines the magnon energy reads:

$$E(k) = E_k = 2\sigma\sqrt{a(k)^2 - b(k)^2} = 2\sigma\,\varepsilon(k) \tag{13}$$

The presence of the magnetization in this expression indicates that the magnon energy is temperature dependent and tends to zero as $T \to T_N$.

Now, choosing the operator $\hat{Q}_m$ to be $\hat{S}_n^-(A)$, one obtains the following GFs:

$$G(k,E) = \left\langle\left\langle \hat{S}^+(A)\,|\,\hat{S}^-(A)\right\rangle\right\rangle_{k,E} = \frac{i}{2\pi}\frac{\sigma}{E_k}\left[\frac{E_k + A_k}{E - E_k} + \frac{E_k - A_k}{E + E_k}\right] \tag{13a}$$

$$\Gamma(k,E) = \left\langle\left\langle \hat{S}^-(B)\,|\,\hat{S}^-(A)\right\rangle\right\rangle_{k,E} = -\frac{i}{2\pi}\frac{\sigma B_k}{E_k}\left[\frac{1}{E - E_k} - \frac{1}{E + E_k}\right] \tag{13b}$$

Making use of the spectral theorem, we may determine the required spin correlation functions. As a reminder, the spectral theorem, according to [45], gives the expectation value of two operators product and reads:

$$\left\langle\hat{B}\hat{A}\right\rangle = \lim_{\varepsilon\to 0^+}\int_{-\infty}^{+\infty} d\omega\,\frac{\left\langle\left\langle \hat{A}\,|\,\hat{B}\right\rangle\right\rangle_{\omega+i\varepsilon} - \left\langle\left\langle \hat{A}\,|\,\hat{B}\right\rangle\right\rangle_{\omega-i\varepsilon}}{e^{\beta\omega} - 1}, \quad \beta = 1/k_B T. \tag{14}$$

a) Magnetization. Since we know the magnon spectrum of the system, it is possible to find the sublattice magnetization. To that end, we need the

correlation function $\left\langle \hat{S}^{-}\hat{S}^{+} \right\rangle$ which may be determined by making use of the GF (13a) and the spectral theorem (14). Thus, we obtain

$$\left\langle \hat{S}^{-}\hat{S}^{+} \right\rangle = 2\sigma\left(\frac{1}{N}\sum_{k} \frac{a_k}{2\varepsilon(k)} \coth\frac{E(k)}{2T} - \frac{1}{2} \right) \equiv 2\sigma\, \Phi(T), \quad (15)$$

where the function $\Phi = \Phi(T)$ is defined as

$$\Phi(T) = \frac{1}{2N}\left(\sum_{k} \frac{a(k)}{\varepsilon(k)} \coth\frac{E(k)}{2T} - 1 \right). \quad (16)$$

Further, we use the Callen self-consistent expression for the mean value of the arbitrary spin S in RPA [45,53]:

$$\sigma = \frac{(S-\Phi)(1+\Phi)^{2S+1} + (S+1+\Phi)\Phi^{2S+1}}{(1+\Phi)^{2S+1} - \Phi^{2S+1}} \quad (17)$$

In the special case when $S = 1$, using expressions (15), (16) and (17), the magnetization becomes:

$$\sigma(T) \equiv \sigma = \frac{1+2\Phi(T)}{1+3\Phi(T)+3\Phi(T)^2} \quad (18)$$

At low temperatures, that is for $T \to 0^{+}$, $\coth\frac{E(k)}{2T} \to 1$ and we have

$$\sigma(T=0K) \equiv \sigma_0 = \frac{1+2\Phi(0)}{1+3\Phi(0)+3\Phi(0)^2}, \quad (19)$$

where

$$\Phi(0) = \frac{1}{2N}\left(\sum_{k} \frac{a(k)}{\varepsilon(k)} - 1 \right). \quad (20)$$

We observe (Eq. (19)) that the sublattice magnetization is finite in the ground state, which will be later also shown numerically for the considered case. The existence of the ground state magnetization lower than the maximal value $\sigma = 1$ indicates that the Neel state is not the ground state for the quantum HAFM.

b) Spin gap. Since we have derived the analytical expressions for the magnon spectrum and the sublattice magnetization, we shall now find the limit when $k \to 0$ in Eq (13). Thus we obtain for the spin spectrum gap the following expression:

$$E(k \to 0, \eta) \equiv \Delta(\eta) = 2\sigma\sqrt{(\eta-1)(J_{1a} - J_{1b} + J_c)[(\eta+1)(J_{1a}+J_c) + (1-\eta)J_{1b} + 4J_2]} \quad (21)$$

wherefrom we conclude that the spin gap depends on the temperature and the spin anisotropy. In the special case when the spin anisotropy is absent, that is $\eta = 1$, the spin gap vanishes. Therefore, we may conclude that the presence of the spin anisotropy is crucial for the gap existence.

In the case of the in-plane isotropy, when $J_{1a} = J_{1b} = J_1$, the gap differs from zero:

$$\Delta(\eta) = 2\sigma\sqrt{(\eta-1)J_c[(\eta+1)J_c + 2J_1 + 4J_2]} \neq 0 \quad (21a)$$

Similarly, in the case when all three NN interactions are equal, that is $J_c = J_{1b} = J_{1a} = J_1$, the gap does not vanish:
$\Delta(\eta) = 2\sigma\sqrt{(\eta-1)J_1[(\eta+3)J_1 + 4J_2]} \neq 0$. We also notice that $\Delta(\eta) \neq 0$ in the absence of the NNN exchange interaction J_2. From Eq. (21a) it is obvious that in case of 2D structure, when the interplanar interaction equals zero (J_c=0), the spin gap vanishes. This suggests that the three-dimensionality is fundamental for the existence of the gap. The detailed analysis of the spin gap for the various system parameters will be performed in Sec. 4.

c) Neel temperature. Since we have derived the expression for the magnetization of the system in the whole temperature interval (Eq. (18)), we shall find the Neel temperature T_N of the system, by making use of the fact that when $T \to T_N$, $\sigma \to 0$. Then the function (16) may be expanded into series in powers of $E(k)/2T << 1$

$$\Phi(T \to T_N) = \frac{1}{N}\sum_{k} \frac{a(k)}{\varepsilon(k)} \frac{k_B T_N}{2\sigma\varepsilon(k)} \quad (22)$$

where we have retained only the first term in the expansion. On the other hand, since in this case $\Phi(T_N)^{-1} \propto \sigma$ is small, the expansion in powers of $\Phi^{-1} \propto \sigma$ may be performed in Eq. (17) [45, 53]:

$$\sigma = \frac{S(S+1)}{3}\Phi^{-1} - \frac{S(S+1)}{6}\Phi^{-2} + \frac{S(S+1)}{3}\frac{9-2S-2S^2}{30}\Phi^{-3} - \ldots \quad (23)$$

Inserting S=1 and combining last two expressions, whereby in Eq. (23) we keep only the first term in the expansion, we obtain the following analytical expression for the Neel temperature within the RPA approach:

$$T_N(\eta) = \frac{4}{3k_B}\left(\frac{1}{N}\sum_{k} \frac{a(k)}{a(k)^2 - b(k)^2} \right)^{-1} \quad (24)$$

This expression, which will be used for the numerical calculations of the critical temperature, shows that the Neel temperature depends on the spin anisotropy and the exchange integrals.

3. LINEAR SPIN-WAVE THEORY

The spin formalism together with the Tyablikov RPA approach presents a powerful and

efficient method, which gives a satisfactory description of the AFM phase in the whole temperature region. However, due to this approximation, a certain error is made, the magnitude of which is almost impossible to estimate. Therefore, it is desirable to examine the considered system also within some other theoretical approach, in order to compare the results.

Most alternative approaches are based on the replacement of the original spin operators with the Bose operators, which have much simpler kinematics. Besides, the Fourier transforms of the Bose operators satisfy the same commutation relations as the Bose operators in the direct space. Among several boson representations which may be used, we choose the linearized Holstein-Primakoff (HP) transformation [45,53]. In this representation, the spin operators on different sublattices read:

$$\hat{S}_i^+(A)=\sqrt{2S}\sqrt{1-\frac{\hat{a}_i^+\hat{a}_i}{2S}}\,\hat{a}_i\cong\sqrt{2S}\,\hat{a}_i,\quad \hat{S}_i^-(A)=\sqrt{2S}\hat{a}_i^+\sqrt{1-\frac{\hat{a}_i^+\hat{a}_i}{2S}}\cong\sqrt{2S}\,\hat{a}_i^+,\quad \hat{S}_i^z(A)=S-\hat{a}_i^+\hat{a}_i$$
$$\hat{S}_i^+(B)=\sqrt{2S}\sqrt{1-\frac{\hat{b}_i^+\hat{b}_i}{2S}}\,\hat{b}_i\cong\sqrt{2S}\,\hat{b}_i,\quad \hat{S}_i^-(B)=\sqrt{2S}\hat{b}_i^+\sqrt{1-\frac{\hat{b}_i^+\hat{b}_i}{2S}}\cong\sqrt{2S}\,\hat{b}_i^+,\quad \hat{S}_i^z(B)=S-\hat{b}_i^+\hat{b}_i \tag{25}$$

The operators $\hat{a}_i^+$ ($\hat{b}_i^+$) and $\hat{a}_i$ ($\hat{b}_i$) present creation and annihilation Bose operators respectively, satisfying for the sublattice A commutation relations:

$$[\hat{a}_i,\hat{a}_j^+]=\delta_{ij},\quad [\hat{a}_i,\hat{a}_j]=[\hat{a}_i^+,\hat{a}_j^+]=0 \tag{26}$$

and analogous relations for the sublattice B. Using the commutation relations (26), it is simple to show that the operators $\hat{S}_i^+(\alpha),\hat{S}_i^-(\alpha)$ and $\hat{S}_i^z(\alpha)$ defined by Eq. (2a) satisfy the commutation relations (2b). The main shortcoming of the boson representations, in general, lies in the fact that the spin operators $\hat{S}_i^-(\alpha)$ and $\hat{S}_i^+(\alpha)$ can create/annihilate only finite number of excitations at the given lattice site, while for the Bose operators that number belongs to the range of values from 0 to ∞. The states with the mean particle number $\langle\hat{a}_i^+\hat{a}_i\rangle>2S$, though mathematically allowed, are not physical. Therefore, it is justified to replace the spin operators by the boson ones as long as the condition $\langle\hat{a}_i^+\hat{a}_i\rangle\le 2S$ is satisfied. This implies that the applicability of the boson approaches raises in the case of low temperatures (the number of excitations per site is small) and/or large spins. Since we are interested in the magnetization and the spin-wave spectrum at the zero temperature when only the quantum fluctuations are present, the Bose operators are expected to be a satisfying approximation of the spin operators.

From Eq. (25), it is obvious that the HP representation is presented by the infinite series in Bose operators, due to the presence of the square root. However, within this paper, we shall keep only the first term in the expansion, which presents the linear or so-called Bloch's approximation. Therefore, after the bosonisation of the Hamiltonian (4c), only the quadratic terms in Bose operators will survive. That means that we ignore the processes of the spin waves scattering, wherefore the approximation is often referred to as the linear spin-wave (LSW) approximation. Thus, after Eqs. (25) are substituted into Hamiltonian (4c), we obtain

$$\begin{aligned}\hat{H}_B=&E_0^{clas}+2SJ_{1a}\sum_n\left[\left(\hat{a}_n^+\hat{b}_{n+\lambda_1^x}^+ +h.c.\right)+\eta\left(\hat{a}_n^+\hat{a}_n+\hat{b}_{n+\lambda_1^x}^+\hat{b}_{n+\lambda_1^x}\right)\right]+\\&+2SJ_{1b}\sum_n\left[\left(\hat{a}_n^+\hat{a}_{n+\lambda_1^y}+\hat{b}_n^+\hat{b}_{n+\lambda_1^y}\right)-\eta\left(\hat{a}_n^+\hat{a}_n+\hat{b}_n^+\hat{b}_n+\hat{a}_{n+\lambda_1^x}^+\hat{a}_{n+\lambda_1^x}+\hat{b}_{n+\lambda_1^x}^+\hat{b}_{n+\lambda_1^x}\right)\right]+\\&+2SJ_c\sum_n\left[\left(\hat{a}_n^+\hat{b}_{n+\lambda_1^z}^+ +h.c.\right)+\eta\left(\hat{a}_n^+\hat{a}_n+\hat{b}_{n+\lambda_1^z}^+\hat{b}_{n+\lambda_1^z}\right)\right]+4SJ_{1a}\sum_n\left[\left(\hat{a}_n^+\hat{b}_{n+\lambda_2}^+ +h.c.\right)+\hat{a}_n^+\hat{a}_n+\hat{b}_{n+\lambda_2}^+\hat{b}_{n+\lambda_2}\right]\end{aligned} \tag{27}$$

where E_0^{clas} presents the ground state energy given by the expression $E_0^{clas}=-2S^2\eta(J_{1a}-J_{1b}+J_c)N-4S^2J_2N.$

Introducing the Fourier transforms

$$\hat{a}_n=\frac{1}{\sqrt{N}}\sum_k\hat{a}_k e^{ikn},\quad \hat{a}_n^+\frac{1}{\sqrt{N}}\sum_k\hat{a}_k^+e^{-ikn} \tag{28}$$

and analogous ones for $\hat{b}_n^{(+)}$, where N signifies the number of magnetic ions in the sublattice A(B), the Hamiltonian (27) becomes:

$$\hat{H}_B=E_0^{clas}+\sum_n\left[A_k^B\left(\hat{a}_k^+\hat{a}_k+\hat{b}_k^+\hat{b}_k\right)+B_k^B\left(\hat{a}_k^+\hat{b}_{-k}^++\hat{a}_k\hat{b}_{-k}\right)\right] \tag{29}$$

Here the quantities A_k^B and B_k^B are the same as in the Eq. (11) with the magnetization σ replaced by the spin S, i.e.

$$A_k^B = 2S\left[(J_{1a} - J_{1b} + J_c)\eta + J_{1b}\cos ak_y + 2J_2\right] = 2S\,a^{(B)}(k)$$
$$B_k^B = 2S\left[J_{1a}\cos ak_x + J_c\cos ak_z + 2J_2\gamma_{2k}\right] = 2S\,b^{(B)}(k) \quad (30)$$

Now we form the equations of motion for the two-time temperature GFs as in Sec. 2:

$$G_k^B(t) = \left\langle\left\langle \hat{a}_k(t) \mid \hat{a}_k^+(0)\right\rangle\right\rangle = \int_{-\infty}^{+\infty} d\omega\, e^{-i\omega t}\left\langle\left\langle \hat{a}_k \mid \hat{a}_k^+\right\rangle\right\rangle_\omega \quad (31)$$

The initial point are the equations of motion for the operators $\hat{a}_k$ and $\hat{b}_{-k}^+$:

$$i\frac{d\hat{a}_k}{dt} = [\hat{a}_k, \hat{H}] = A_k^B\hat{a}_k - B_k^B\hat{b}_{-k}^+ \quad (32)$$

$$i\frac{d\hat{b}_{-k}^+}{dt} = [\hat{b}_{-k}^+, \hat{H}] = -B_k^B\hat{a}_k - A_k^B\hat{b}_{-k}^+ \quad (33)$$

where the commutator is to be determined using the Hamiltonian (29).

The system of equations for the corresponding GFs reads:

$$\begin{aligned}\left(E - A_k^B\right)\left\langle\left\langle \hat{a}_k \mid \hat{a}_k^+\right\rangle\right\rangle_{k,E} - B_k^B\left\langle\left\langle \hat{b}_{-k}^+ \mid \hat{a}_k^+\right\rangle\right\rangle_{k,E} &= \frac{i}{2\pi}\\ B_k^B\left\langle\left\langle \hat{a}_k \mid \hat{a}_k^+\right\rangle\right\rangle_{k,E} + \left(E + A_k^B\right)\left\langle\left\langle \hat{b}_{-k}^+ \mid \hat{a}_k^+\right\rangle\right\rangle_{k,E} &= 0\end{aligned} \quad (34)$$

Solving this algebraic system of equations we find the following GFs:

$$\begin{aligned}\left\langle\left\langle \hat{a}_k \mid \hat{a}_k^+\right\rangle\right\rangle_{k,E} &= \frac{i}{2\pi}\frac{1}{2E_k}\left[\frac{E_k^B + A_k^B}{E - E_k^B} + \frac{E_k^B - A_k^B}{E + E_k^B}\right]\\ \left\langle\left\langle \hat{b}_{-k}^+ \mid \hat{a}_k^+\right\rangle\right\rangle_{k,E} &= \frac{i}{2\pi}\frac{B_k^B}{E^2 - \left(E_k^B\right)^2}\end{aligned} \quad (35)$$

The magnon spectrum within the LSW theory reads:

$$E^{(B)}(k) = E_k^{(B)} = 2S\sqrt{a^{(B)}(k)^2 - b^{(B)}(k)^2} = 2S\,\varepsilon^{(B)}(k) \quad (36)$$

By inspection of Eq. (36) it is easy to notice that the elementary excitation spectrum within the LSW theory does not differ from the RPA one, except for the fact that the magnetization σ in Eq. (13) is here replaced by the spin S (in special case considered in the paper S=1).

a) Magnetization**.** Within the LSW theory, the sublattice magnetization is defined by the following expression (since the magnetizations on two sublattices do not differ, it is sufficient to consider one sublattice, A for instance):

$$\left\langle\hat{S}_n^z(A)\right\rangle = \left\langle\hat{S}^z\right\rangle \equiv \sigma = S - \left\langle\hat{a}_n^+\hat{a}_n\right\rangle = S - \frac{1}{N}\sum_k\left\langle\hat{a}_k^+\hat{a}_k\right\rangle \quad (37)$$

In order to find the correlation function, $\left\langle\hat{a}_k^+\hat{a}_k\right\rangle$ we use the spectral theorem (14). Therefore, we need the GF $\left\langle\left\langle \hat{a}_k \mid \hat{a}_k^+\right\rangle\right\rangle$, already calculated in (35). Hence,

$$\left\langle\hat{a}_k^+\hat{a}_k\right\rangle = \frac{1}{2}\left(\frac{a^{(B)}(k)}{\varepsilon^{(B)}(k)}\coth\frac{E^{(B)}(k)}{2k_BT} - 1\right). \quad (38)$$

Finally, the sublattice magnetization reads:

$$\left\langle\hat{S}_n^z(A)\right\rangle = \left\langle\hat{S}^z\right\rangle \equiv \sigma = S - \frac{1}{2N}\sum_k\left(\frac{a^{(B)}(k)}{\varepsilon^{(B)}(k)}\coth\frac{E^{(B)}(k)}{2k_BT} - 1\right) = S + \frac{1}{2} - \frac{1}{2N}\sum_k\frac{a^{(B)}(k)}{\varepsilon^{(B)}(k)}\coth\frac{E^{(B)}(k)}{2k_BT} \quad (39)$$

This expression will be analyzed numerically in the following Section.

Since we consider the ground state of the system, where $\coth\frac{E^{(B)}(k)}{2k_BT} \to 1$, the magnetization (39) at $T = 0K$ becomes

$$\left\langle\hat{S}^z\right\rangle_0 \equiv \sigma_0 = S + \frac{1}{2} - \frac{1}{2N}\sum_k\frac{a^{(B)}(k)}{\varepsilon^{(B)}(k)} \quad (40)$$

b) Spin gap. Using the magnon spectrum given by Eq. (36), we may determine the spin gap within the LSW theory. Therefore, we look for the limit when $k \to 0$ in (36) and obtain:

$$E^{(B)}(k \to 0, \eta) \equiv \Delta^{(B)}(\eta) = 2S\sqrt{(\eta - 1)(J_{1a} - J_{1b} + J_c)[(\eta + 1)(J_{1a} + J_c) + (1 - \eta)J_{1b} + 4J_2]} \quad (41)$$

From this expression, it is obvious that the spin gap does not depend on temperature, while the spin anisotropy dependence is the same as within the RPA approach, wherefore the same remarks and conclusions considering the importance of the spin anisotropy for the existence of the spin gap may be drawn.

In the isotropic case, when $J_{1a} = J_{1b} = J_1$, the spin gap equals $\Delta^{(B)}(\eta) = 2S\sqrt{(\eta - 1)J_c[2J_1 + (\eta + 1)J_c + 4J_2]} \neq 0$. For $J_{1a} = J_{1b} = J_c = J_1$ the spin gap has non-zero value as well: $\Delta^{(B)}(\eta) = 2S\sqrt{(\eta - 1)J_1[(\eta + 3)J_1 + 4J_2]} \neq 0$. The analogous conclusion may also be drawn in the case when the NNN exchange interaction is absent.

4. COMPARISON TO THE EXPERIMENTAL DATA AND DISCUSSION

In previous sections we have derived the analytical expressions for the magnetization, Neel temperature and the spin gap for the 1111-type compounds with arbitrary spin within the RPA and LSW theory approach. Now we shall perform the numerical analysis of the obtained expressions. We have shown that these quantities depend on the temperature and the parameters of our model, primarily exchange integrals and the spin anisotropy. However, the agreement has not been achieved yet concerning the values of the exchange integrals, due to the ambiguous microscopic origin of this kind of AFM order. The type of the magnetic anisotropy has not been fully clarified yet as well.

Some papers suggest that in the 1111-type compounds local or single-ion magnetic anisotropy is present, due to their layered structure. It is considered to originate from the presence of the subsystem of the rare earth elements (La, Ce, Pr, Nd, Sm,…) on the one hand and the subsystem of the iron with the *3d* electrons on the other. The interaction of these two subsystems certainly brings about effective anisotropy, the type of which, nevertheless, has not been solved so far. This problem merits attention and requires subtle study of the anisotropic properties of these two subsystems in ferropnictides. In this paper, we have considered *the spin anisotropy* in the FeAs planes within the effective AFM Heisenberg model. We shall use the estimated exchange integrals values in undoped LaOFeAS from existing literature [49,50]: $J_{1a}=50\pm10meV$, $J_{1b}=49\pm10meV$, $J_c=0.020\pm0.015meV$ and $J_2=26\pm5meV$. The numerical calculations will be performed with the spin quantum number $S=1$. Since we have chosen to analyze the systems with the spin anisotropy $\eta=1+\delta\geq1$, we shall vary this parameter in the obtained analytical expressions (especially that for the Neel temperature $T_N(\eta)$) in order to obtain the experimental value for the critical temperature.

Our calculations of the critical temperature T_N within the proposed anisotropic 3D model are based on the analytical RPA expression (24). For the aforementioned set of the exchange integrals, the spin anisotropy parameter which reproduces the experimental value of the critical temperature ($T_N^{\exp}=137K$), reads $\eta=1.0303$. The Neel temperature dependence on the various spin anisotropy parameter values $\eta\geq1$ for the specified set of the exchange integrals is presented in Figure 3.

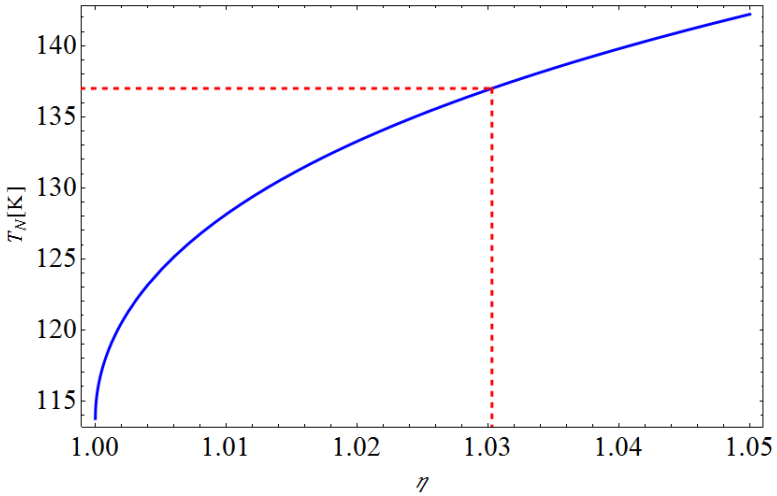

Figure 3. The critical temperature dependence on the spin anisotropy parameter. Exchange integrals are specified in the text. The dotted lines intersection corresponds to the spin anisotropy parameter value $\eta=1.0303$ which reproduces the experimental critical temperature T_N=137K. The spin of the system is unity (S=1).

The Figure shows that the Neel temperature is monotonically increasing function of the spin anisotropy parameter. In the absence of the spin anisotropy ($\eta=1$), we have obtained the critical temperature T_N=113.75 K, in disaccord with the results from [49]. Having in mind that the authors in that paper examined the same model (except without anisotropy) within the same (GF) method, we assume that the mentioned discrepancy originates from the numerical calculations.

Further, we examine the Neel temperature dependence on the intra-layer exchange integral J_c. The results of the corresponding numerical calculations are plotted in Figure 4.

We show the critical temperature dependence on the intra-layer exchange integral both in the

absence of the spin anisotropy in the model Hamiltonian ($\eta = 1$) and for the spin anisotropy value which reproduces correctly the experimental value of T_N ($\eta = 1.0303$). It is obvious from the Figure that the Neel temperature grows with the increase in J_C. This growth is slower in the presence of the spin anisotropy. Finally, let us note that the parameter values $J_c = 0, \eta = 1$ correspond to the isotropic 2D Heisenberg AFM. In that case T_N=0, in agreement with the Mermin-Wagner theorem, according to which a one- or two-dimensional isotropic spin-S Heisenberg model with finite-range exchange interactions cannot possess the long range order at any finite temperature [53].

The spin spectrum gap dependence on the spin anisotropy parameter within RPA and LSW approach is plotted in Figure 5.

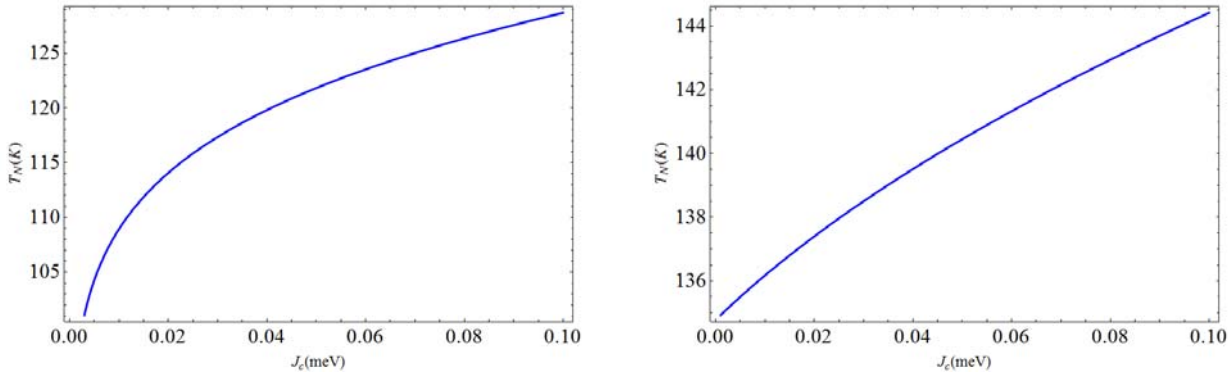

Figure 4. The Neel temperature T_N dependence on the intra-layer exchange integral J_c. Exchange integrals are specified in the text. Left plot presents the case without anisotropy, i.e. $\eta = 1$. The right plot corresponds to $\eta = 1.0303$.

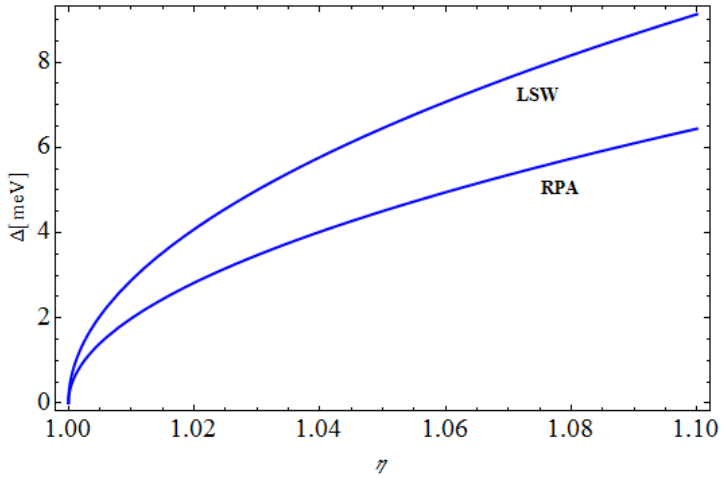

Figure 5. The spin gap dependence on the spin anisotropy parameter at T=0K within RPA and LSW theory. Exchange integrals are specified in the text.

The Figure shows that the spin gap increases with the the anisotropy parameter in the similar way within both approaches. Thereby, the spin gap values within RPA are slightly lower than the corresponding values within LSW theory for all spin anisotropy parameter values $\eta > 1$. Using Eq. (21) within RPA and Eq. (41) within LSW approach, we have performed the numerical calculations of the spin gap including the exchange interactions and the spin anisotropy parameter which reproduce the experimental critical temperature. Thus, we have obtained $\Delta^{3D}_{RPA}(\eta = 1.0303) = 3.49meV$, $\Delta^{3D}_{LSW}(\eta = 1.0303) = 5.02meV$. These values show a satisfactory qualitative agreement with the existing results from the literature [49,50,59].

Finally, we examine the ground state (T=0K) magnetization dependence on the spin anisotropy parameter within RPA and LSW approach. The results of the numerical calculations plotted in Figure 6. show that the ground state magnetization is a monotonically increasing function of the spin anisotropy parameter, whereby the RPA values are slightly higher than the LSW ones. In the special

case when $\eta = 1.0303$ with other parameters unaffected, we have obtained $\sigma_0^{3D}(RPA) = 0.6946$ and $\sigma_0^{3D}(LSW) = 0.6947$. It is obvious that the ground state magnetization is approximately the same within both approaches and less than unity due to the quantum fluctuations. Hence, the quantum fluctuations are in case of the antiferromagnet present at the absolute zero as well. Therefore the Neel state is not the ground state of the antiferromagnet at T=0K.

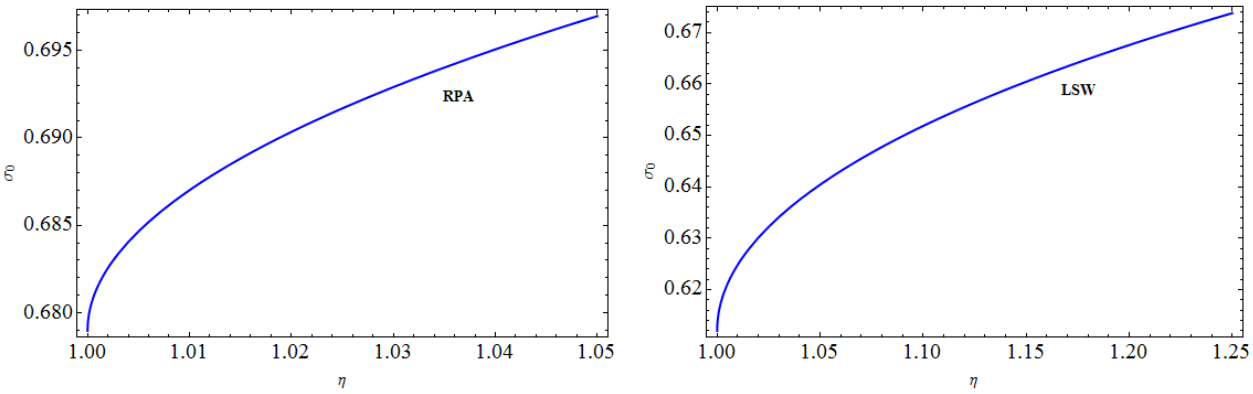

Figure 6. The ground state magnetization dependence on the spin anisotropy parameter. Exchange integrals are specified in the text.

5. CONCLUSION

In this paper, we have examined the thermodynamic properties of the antiferromagnetic ferropnictides of the 1111-type, based on the effective J_{1a}-J_{1b}-J_c-J_2 Heisenberg AFM model with arbitrary spin. We have derived first the expression for the spin-wave spectrum using the two-time temperature Green functions. Thence we have obtained the sublattice magnetization in dependence of the temperature, as well as the explicit formula for the critical temperature T_N within RPA, by making use of the Tyablikov self-consistent decoupling of the higher-order Green functions. We have also derived the corresponding expressions for the magnon spectrum, spin gap and ground state magnetization within the LSW theory.

Special attention has been paid to the layered LaOFeAS, since there exists [2] the experimental result for the Neel temperature in this compound (T_N(LaOFeAS)=137 K). By numerical calculations we have obtained, within the proposed effective anisotropic AFM model, the theoretical value for the critical temperature (T_N(th)). This was achieved by the variation of the spin anisotropy introduced through the parameter $\eta = 1 + \delta \geq 1$. It was shown that the critical temperature is a monotonically increasing function of the spin anisotropy parameter. The parameter value which was found to reproduce the experimentally obtained Neel temperature reads $\eta = 1.0303$. The other model parameters, i.e. the exchange integrals $J_{1a,b}$, J_c and J_2 were taken from the literature [49,50]. Despite the relatively simple model and approximation, there is an excellent agreement between the theoretical and experimental critical temperature. This suggests that *the spin anisotropy is responsible for the magnetic properties of the 1111-ferropnictides family* and presents *a convincing argument in making conclusions about the anisotropy type in these compounds*. Therefore, the proposed model and the self-consistent Tyablikov approximation within the two-time temperature Green functions method turn out to be a perspective approach for the theoretical studies of the AFM properties of the 1111-FeAS compounds.

Further, substituting the value $\eta = 1.0303$ in the analytical expression for the spin gap spectrum, we were able to calculate numerically the spin gap within the used approach. We obtained that the spin gap at low temperatures is of the order of magnitude of several meV, in a satisfactory qualitative agreement with the experimental results for the ferropnictides family [59]. Let us emphasize that within the LSW theory we got slightly higher values for the spin gap than the RPA ones, which was expected due to the fact that the gap was calculated at low temperatures (close to $T \to 0^+$). It is well-known that in that case the LSW theory presents a good approximation for the magnon spectrum and thus also for the corresponding spin gap. The temperature dependence of the spin gap is determined by the magnetization which enters the expression for the spin gap within RPA. It is clear that within this approximation, the gap tends to zero when the tem-

perature is increased and tends to T_N. On the contrary, within LSW theory, the gap does not depend on temperature and has a constant value within the whole temperature region.

Finally, let us conclude that the GF method may be successfully applied to a broad class of ferropnictides. The results of these analyses should, among the rest, be helpful in the attempts of understanding the physical, especially superconducting properties of these compounds.

6. ACKNOWLEDGMENT

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УТИЦАЈ АНИЗОТРОПИЈЕ НА ПРУГАСТИ ФРУСТРИРАНИ ХАЈЗЕНБЕРГОВ АНТИФЕРОМАГНЕТНИ МОДЕЛ: ПРИМЕНА НА ПНИКТИДЕ ГВОЖЂА

Сажетак: Изучавамо термодинамичка својства једињења пниктида гвожђа у оквиру анизотропног J_{1a} - J_{1b} - J_c - J_2 Хајзенберговог антиферомагнетног модела, мотивисани бројним експерименталним студијама ових једињења. Наше калкулације базирамо на методу двовременских температурских Гринових функција у оквиру добро познатих апроксимација. Налазимо магнонски ексцитациони спектар, корелационе функције и аналитички израз за критичну температуру и поредимо наше резултате са постојећим експерименталним подацима. Резултати добијени у овом раду могу бити од великог значаја за будућа истраживања сличних магнетних система.

Кључне речи: фрустрирани Хајзенбергов J_{1a} - J_{1b} - J_c - J_2 антиферомагнет, пниктиди гвожђа, спинска анизотропија, пругаста спинска фаза, Нелова температура.