Original scientific paper

UDK 620.178.2:669.15-194.2
DOI 10.7251/COMEN2202195A

TRANSITION TEMPERATURE DEPENDENCE ON ANISOTROPY IN THE J_1-J_2-J_c-J_p HEISENBERG MODEL WITH APPLICATION TO 122-TYPE OF IRON PNICTIDES

Miloš Adamović,[1*] Milan Pantić[2]

[1] University of Kragujevac, Faculty of Science, Kragujevac, Serbia
[2] University of Novi Sad, Faculty of Sciences, Novi Sad, Serbia
[*] Corresponding author: milos.adamovic@pmf.kg.ac.rs

Abstract: Recently there has been a considerable interest in studying iron-based superconductors called pnictides. The aim of this paper is to give a contribution to better understanding of magnetic properties of the 122 class of iron pnictides. We use anisotropic J_1-J_2-J_c-J_p Heisenberg model. The method of spin Green's functions in the Tyablikov's random phase approximation (RPA) decoupling scheme is used to determine the transition temperature. Based on the obtained expression for the transition temperature, we study its dependence on the spin anisotropy. Furthermore, we compare our model results with the experimentally available data for the transition temperature. In addition, we test our model predictions of the transition temperature using the exchange interaction values from other articles. Results presented here should give additional contribution to understanding the magnetic properties of the 122 class of iron-based superconductors.

Keywords: Neel temperature, spin anisotropy, iron pnictides, anisotropic Heisenberg model

1. INTRODUCTION

The discovery of superconductivity in fluorine-doped LaOFeAs opened a new direction in the research of unconventional high-temperature superconductors [1]. It was followed by numerous, both theoretical and experimental, studies of a newly discovered class of iron-based superconductors, called pnictides. Today, the family of high-temperature iron-based superconductors includes pnictides such as the so-called 1111-system RFeAsO (R-rare Earth element), 122-system AFe_2As_2 (A = Ba, Ca, Sr), 111-system XFeAs (X = Li) and 11-system such as FeSe [2-7]. New types of iron-based superconductors are even recently being discovered such as the so-called 1144 class [8] and new research is done constantly on previously discovered compounds [9]. Pnictides showed a lot of similarities with the so-called cuprates, a well-studied class of high-temperature superconductors [10]. The main similarity between cuprates and pnictides is the layered structure (see Figure 1). In the case of pnictides the layered structure is made by layers of FeAs. Pnictides, like the cuprates, have a long-range magnetic order that is lost by doping with electrons or holes, when a superconducting state occurs.

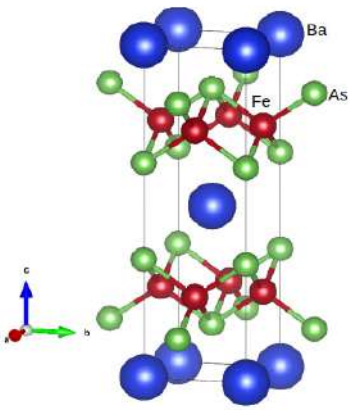

Figure 1. *Crystal structure of $BaFe_2As_2$, an iron pnictide compound of the 122-type in undoped regime*

Undoped pnictide compounds are bad metals that have a long-range antiferromagnetic order below the Neel temperature $T_N \leq 220$ K [11,12]. Although it is believed that magnetism has a significant role in the onset of superconductivity in pnictides, there is still no general accordance on the magnetic interactions in these compounds. There are currently two active ways of looking at the nature of magnetism in pnictides: model of localized electrons and itinerant model. In this paper, we present the results of modeling the 122 pnictide system as a system of localized electrons within the anisotropic Heisenberg antiferromagnetic model. We will use the 3D anisotropic Heisenberg antiferromagnetic J_1-J_2-J_c-J_p model to calculate the spin-wave spectrum and from it derive the transition (Neel, critical) temperature T_N. Above this temperature long-range magnetic order in destroyed. Similar work was done on the analysis of 1111-system of pnictides in undoped phase [13]. Main idea of this paper is to give the selection of magnetic interactions that are used in model spin Hamiltonian and to see how Neel temperature depends on them and on spin anisotropy.

This work is organized as follows: after general introduction we will give an overview of three-dimensional antiferromagnetic J_1-J_2-J_c-J_p Heisenberg model with spin anisotropy. By using the Green's function method for spin operators, we will obtain spin-wave spectrum and Neel temperature. Green's functions equations of motion are decoupled by using so-called Tyablikov's decoupling or random phase approximation. After that, we will present numerical results that will show how does Neel temperature depend on model parameters, anisotropy and how results compare with the experimental data. Finally, we summarize the conclusions and give an overview of used literature.

2. MODEL HAMILTONIAN AND MAIN RESULTS

In order to describe antiferromagnetic long-range order of layered 122-type of pnictides we use Heisenberg model on a bilayer magnetic unit cell. We use the following Hamiltonian:

$$\begin{aligned}\hat{H} = \sum_{m\vec{\rho}}\sum_{i=1}^{2}\Bigg(\sum_{\vec{\lambda_\alpha}} J_{1\alpha}\left(\hat{\vec{S}}_{m\vec{\rho}}(a_i)\hat{\vec{S}}_{m\vec{\rho}+\vec{\lambda_\alpha}}(b_i) + \hat{\vec{S}}_{m\vec{\rho}}(A_i)\hat{\vec{S}}_{m\vec{\rho}+\vec{\lambda_\alpha}}(B_i)\right)\Bigg) \\ + \sum_{m\vec{\rho}} J_c(\hat{\vec{S}}_{m\vec{\rho}}(a_1)\hat{\vec{S}}_{m\vec{\rho}}(b_2) + \hat{\vec{S}}_{m\vec{\rho}}(b_1)\hat{\vec{S}}_{m\vec{\rho}}(a_2) + \hat{\vec{S}}_{m\vec{\rho}}(A_1)\hat{\vec{S}}_{m\vec{\rho}}(B_2) + \hat{\vec{S}}_{m\vec{\rho}}(B_1)\hat{\vec{S}}_{m\vec{\rho}}(A_2)) \\ + \sum_{m\vec{\rho}} J_p\,(\hat{\vec{S}}_{m\pm1,\vec{\rho}}(a_1)\hat{\vec{S}}_{m\pm1,\vec{\rho}}(b_2) + \hat{\vec{S}}_{m\pm1,\vec{\rho}}(b_1)\hat{\vec{S}}_{m\pm1,\vec{\rho}}(a_2) + \hat{\vec{S}}_{m\pm1,\vec{\rho}}(A_1)\hat{\vec{S}}_{m\pm1,\vec{\rho}}(B_2) \\ + \hat{\vec{S}}_{m\pm1,\vec{\rho}}(B_1)\hat{\vec{S}}_{m\pm1,\vec{\rho}}(A_2)) + \sum_{m\vec{\rho}}\sum_{\vec{\lambda_2}}\sum_{i=1}^{2} J_2\,(\hat{\vec{S}}_{m\vec{\rho}}(a_i)\hat{\vec{S}}_{m\vec{\rho}+\vec{\lambda_2}}(B_i) + \hat{\vec{S}}_{m\vec{\rho}}(b_i)\hat{\vec{S}}_{m\vec{\rho}+\vec{\lambda_2}}(A_i))\end{aligned} \quad (1)$$

where $\hat{\vec{S}}_{m\vec{\rho}}(n_i)$ represents spin operators in the n_i-th sublattice in the m-th bilayer, while $\vec{\rho}$ is the position of spin inside bilayer plane and $\alpha = a, b$. Figure 2 shows magnetic elementary cell with eight sublattices labeled by $n_i = a_i, b_i, A_i, B_i$ for $i = 1,2$.

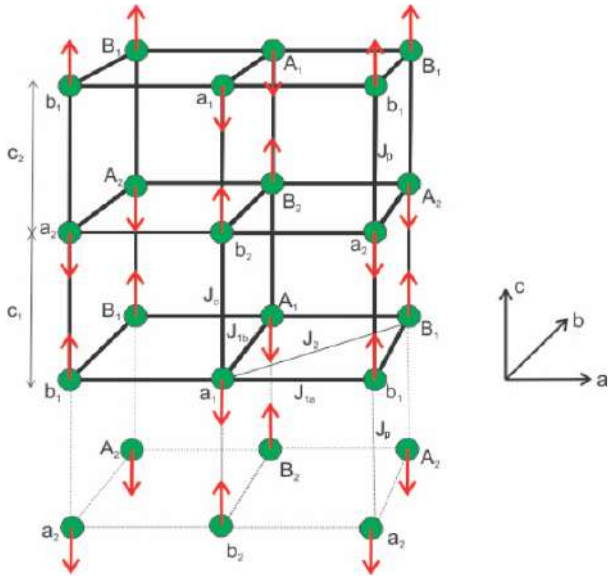

Figure 2. *Magnetic unit cell of a bilayer used to model 122-type of pnictides with the dominant spin interactions labeled*

Nearest neighbors along directions a and b are denoted by $\vec{\lambda}_{a/b}$ while J_{1a} and J_{1b} will be corresponding exchange integrals [9,11,14-17]. Next nearest neighbors are labeled as $\vec{\lambda}_2$ with its corresponding integral J_2. Exchange integral of spins between layers in bilayer is denoted by J_c and interaction between different bilayers is J_p [18,19]. Interactions between layers and bilayers are taken to be a lot weaker than the other ones. The effect of structural phase transition will be omitted, although it was observed in pnictide compounds, so the used elementary cell will be tetragonal. The exchange integrals are assumed to be antiferromagnetic if J>0 and ferromagnetic if J<0. Spin operators $\hat{S}^x(n_i)$, $\hat{S}^y(n_i)$, $\hat{S}^z(n_i)$ are expressed in terms of raising and lowering spin operators $\hat{S}^{\pm}(n_i)$ [20]. Spin anisotropy is taken into account along z-direction for interactions given by exchange integrals J_{1a}, J_{1b}, J_c and it is given by parameter η (η=1+δ, δ<<1). In order to make our calculations and analysis a bit easier, a rotation by π is done in spin space for sublattices $n' = a_2, b_1, A_2, B_1$. In other words, new local coordinate system is introduced which is done by unitary transformation of spin operators on lattice points that correspond to sublattices *n'* [21]. Introduced magnetic unit cell shows striped order of spins and for that it should be taken that $J_2 > J_{1a}/2$. Also, all exchange integrals are taken to be positive except J_{1b} (will be negative, but can be taken positive as well). Calculations are done within the Green's functions formalism for the arbitrary spin value S, and specifically for the S=1 [12,22]. We are using method of double-time temperature Green's functions [23]. Equations of motion for the Green's functions of operators $\hat{S}^+_{m\vec{\rho}}(a_1)$, $\hat{S}^-_{m\vec{\rho}}(b_1)$, $\hat{S}^+_{m\vec{\rho}}(A_1)$, $\hat{S}^-_{m\vec{\rho}}(B_1)$, $\hat{S}^+_{m\vec{\rho}}(a_2)$, $\hat{S}^-_{m\vec{\rho}}(b_2)$, $\hat{S}^+_{m\vec{\rho}}(A_2)$, $\hat{S}^-_{m\vec{\rho}}(B_2)$ are calculated [13,21]. Further calculations were done by using so-called Tyablikov's decoupling or random phase approximation where we have that [23]:

$$\langle\langle \hat{S}_i^z(\beta)\, \hat{S}_l^{\pm}(\gamma) |\, \hat{R}_m(\varepsilon)\rangle\rangle \equiv \langle\langle \hat{S}_i^z(\beta)\rangle\rangle \langle\langle \hat{S}_l^{\pm}(\gamma) |\, \hat{R}_m(\varepsilon)\rangle\rangle, i \neq l \tag{2}$$

Operator $\hat{R}$ can be chosen arbitrarily. Translational invariance and rotation in spin space allow that for every sublattice we can take $\langle \hat{S}^z(\beta)\rangle = \sigma(\beta) \equiv \sigma$ as the ordering parameter, namely, sublattice magnetization. Using appropriate Fourier transformations we get and use:

$$\hat{S}^+_{m\vec{\rho}}(\beta) = \frac{1}{\sqrt{N_2 N_z}} \sum_{\vec{k}} \hat{S}^+_{\vec{k}}(\beta) e^{i\vec{k}_{||}\cdot\vec{\rho} + i(mL + (n_z - 1)a)k_z}, \quad n_z = 1,2 \tag{3}$$

where N_2 is the number of atoms in a-b plane, m counts bilayers, $L=c_1+c_2$ represents period of superlattice along c direction. We obtain the following system of equations for the Green's functions:

$$(\omega-\epsilon)\langle\langle\hat{S}^{+}(a_1)|\hat{R}\rangle\rangle-2J_a\langle\langle\hat{S}^{-}(b_1)|\hat{R}\rangle\rangle-2J_b\langle\langle\hat{S}^{+}(A_1)|\hat{R}\rangle\rangle-4J_d\langle\langle\hat{S}^{-}(B_1)|\hat{R}\rangle\rangle-J_{cc}\langle\langle\hat{S}^{-}(b_2)|\hat{R}\rangle\rangle=\frac{1}{2\pi}\langle[\hat{S}^{+}(a_1),\hat{R}]\rangle \quad (4a)$$

$$2J_a\langle\langle\hat{S}^{+}(a_1)|\hat{R}\rangle\rangle+(\omega+\epsilon)\langle\langle\hat{S}^{-}(b_1)|\hat{R}\rangle\rangle+4J_d\langle\langle\hat{S}^{+}(A_1)|\hat{R}\rangle\rangle+2J_b\langle\langle\hat{S}^{-}(B_1)|\hat{R}\rangle\rangle+J_{cc}\langle\langle\hat{S}^{+}(a_2)|\hat{R}\rangle\rangle=\frac{1}{2\pi}\langle[\hat{S}^{-}(b_1),\hat{R}]\rangle \quad (4b)$$

$$-2J_b\langle\langle\hat{S}^{+}(a_1)|\hat{R}\rangle\rangle-4J_d\langle\langle\hat{S}^{-}(b_1)|\hat{R}\rangle\rangle+(\omega-\epsilon)\langle\langle\hat{S}^{+}(A_1)|\hat{R}\rangle\rangle-2J_a\langle\langle\hat{S}^{-}(B_1)|\hat{R}\rangle\rangle-J_{cc}\langle\langle\hat{S}^{-}(B_2)|\hat{R}\rangle\rangle=\frac{1}{2\pi}\langle[\hat{S}^{+}(A_1),\hat{R}]\rangle \quad (4c)$$

$$4J_d\langle\langle\hat{S}^{+}(a_1)|\hat{R}\rangle\rangle+2J_b\langle\langle\hat{S}^{-}(b_1)|\hat{R}\rangle\rangle+2J_a\langle\langle\hat{S}^{+}(A_1)|\hat{R}\rangle\rangle+(\omega+\epsilon)\langle\langle\hat{S}^{-}(B_1)|\hat{R}\rangle\rangle+J_{cc}\langle\langle\hat{S}^{+}(A_2)|\hat{R}\rangle\rangle=\frac{1}{2\pi}\langle[\hat{S}^{-}(B_1),\hat{R}]\rangle \quad (4d)$$

$$-J_{ccc}\langle\langle\hat{S}^{-}(b_1)|\hat{R}\rangle\rangle+(\omega-\epsilon)\langle\langle\hat{S}^{+}(a_2)|\hat{R}\rangle\rangle-2J_a\langle\langle\hat{S}^{-}(b_2)|\hat{R}\rangle\rangle-2J_b\langle\langle\hat{S}^{+}(A_2)|\hat{R}\rangle\rangle-4J_d\langle\langle\hat{S}^{-}(B_2)|\hat{R}\rangle\rangle=\frac{1}{2\pi}\langle[\hat{S}^{+}(a_2),\hat{R}]\rangle \quad (4e)$$

$$J_{ccc}\langle\langle\hat{S}^{+}(a_1)|\hat{R}\rangle\rangle+2J_a\langle\langle\hat{S}^{+}(a_2)|\hat{R}\rangle\rangle+(\omega+\epsilon)\langle\langle\hat{S}^{-}(b_2)|\hat{R}\rangle\rangle+4J_d\langle\langle\hat{S}^{+}(A_2)|\hat{R}\rangle\rangle+2J_b\langle\langle\hat{S}^{-}(B_2)|\hat{R}\rangle\rangle=\frac{1}{2\pi}\langle[\hat{S}^{-}(b_2),\hat{R}]\rangle \quad (4f)$$

$$-J_{ccc}\langle\langle\hat{S}^{-}(B_1)|\hat{R}\rangle\rangle-2J_b\langle\langle\hat{S}^{+}(a_2)|\hat{R}\rangle\rangle-4J_d\langle\langle\hat{S}^{-}(b_2)|\hat{R}\rangle\rangle+(\omega-\epsilon)\langle\langle\hat{S}^{+}(A_2)|\hat{R}\rangle\rangle-2J_a\langle\langle\hat{S}^{-}(B_2)|\hat{R}\rangle\rangle=\frac{1}{2\pi}\langle[\hat{S}^{+}(A_2),\hat{R}]\rangle \quad (4g)$$

$$J_{ccc}\langle\langle\hat{S}^{+}(A_1)|\hat{R}\rangle\rangle+4J_d\langle\langle\hat{S}^{+}(a_2)|\hat{R}\rangle\rangle+2J_b\langle\langle\hat{S}^{-}(b_2)|\hat{R}\rangle\rangle+2J_a\langle\langle\hat{S}^{+}(A_2)|\hat{R}\rangle\rangle+(\omega+\epsilon)\langle\langle\hat{S}^{-}(B_2)|\hat{R}\rangle\rangle=\frac{1}{2\pi}\langle[\hat{S}^{-}(B_2),\hat{R}]\rangle \quad (4h)$$

where we have used following notation:

$$\epsilon=\sigma((2J_{1a}-2J_{1b}+J_c)\eta+J_p+4J_2) \quad (5a)$$

$$J_a=\sigma J_{1a}\cos(ak_x) \quad (5b)$$

$$J_b=\sigma J_{1b}\cos(ak_y) \quad (5c)$$

$$J_d=\sigma J_2\cos(ak_x)\cos(ak_y) \quad (5d)$$

$$J_{cc}=\sigma(J_c+J_pe^{-ick_z}) \quad (5e)$$

$$J_{ccc}=\sigma(J_c+J_pe^{ick_z}) \quad (5f)$$

Solving system of equations for Green's functions gives us spin wave dispersion.

Spin waves dispersion has four positive solutions:

$$E_1=\sqrt{(\epsilon-2J_b)^2-4(J_a-2J_d)^2-J_{cc}J_{ccc}-4\sqrt{J_{cc}J_{ccc}(J_a-2J_d)^2}} \quad (6a)$$

$$E_2=\sqrt{(\epsilon-2J_b)^2-4(J_a-2J_d)^2-J_{cc}J_{ccc}+4\sqrt{J_{cc}J_{ccc}(J_a-2J_d)^2}} \quad (6b)$$

$$E_3=\sqrt{(\epsilon+2J_b)^2-4(J_a+2J_d)^2-J_{cc}J_{ccc}-4\sqrt{J_{cc}J_{ccc}(J_a+2J_d)^2}} \quad (6c)$$

$$E_4=\sqrt{(\epsilon+2J_b)^2-4(J_a+2J_d)^2-J_{cc}J_{ccc}+4\sqrt{J_{cc}J_{ccc}(J_a+2J_d)^2}} \quad (6d)$$

where E_3 has the Goldstone mode. Spin gap that is obtained when $\vec{k}\to 0$ in E_3 vanishes when η=0. Spin wave dispersion depends on magnetization and that indicates that magnon energy is temperature dependent and tends to zero as $T\to T_N$. In order to obtain sublattice magnetization we have calculated correlation function:

$$\langle\hat{S}^{-}(a_1)\hat{S}^{+}(a_1)\rangle\equiv 2\sigma\Phi(T) \quad (7)$$

where the function Φ is given by:

$$\Phi(T)=\frac{1}{N}\sum_{\vec{k}}\left(\sum_{i=1}^{2}\left(\frac{\epsilon-2J_b}{8E_i}\coth\left(\frac{E_i}{2k_BT}\right)\right)+\sum_{j=3}^{4}\left(\frac{\epsilon+2J_b}{8E_j}\coth\left(\frac{E_j}{2k_BT}\right)\right)-\frac{1}{2}\right) \quad (8)$$

where T is the temperature and k_B is the Boltzmann's constant. Further on, we use the self-consistent

Callen's relation for the magnetization for arbitrary spin S in random phase approximation [20,23]:

$$\sigma = \frac{(S-\Phi)(1+\Phi)^{2S+1} + (S+1+\Phi)\Phi^{2S+1}}{(1+\Phi)^{2S+1} - \Phi^{2S+1}} \quad (9)$$

Magnetization is a function of temperature as well as all the exchange integrals and spin anisotropy (model parameters). We obtain the Neel temperature using that when $T \to T_N$ then $\sigma \to 0$. For the case of S=1 obtained expression for the Neel temperature in random phase approximation is [13,21]:

where for example, in the case of S=1 the magnetization is given with:

$$\sigma = \frac{1+2\Phi(T)}{1+3\Phi(T)+3\Phi^2(T)} \quad (10)$$

where $\tilde{\epsilon} = (2J_{1a} - 2J_{1b} + J_c)\eta + J_p + 4J_2$ and $\tilde{E}_i = E_i/\sigma$ for i=1,2,3,4. In the following section we will use (11) in order to perform numerical analysis of obtained expression and present the influence of anisotropy on Neel temperature.

$$T_N = \frac{2}{3k_B} \frac{1}{\frac{1}{4N}\sum_{\vec{k}} \left(\frac{\tilde{\epsilon} - 2J_{1b}\cos(ak_y)}{\tilde{E}_1^2} + \frac{\tilde{\epsilon} - 2J_{1b}\cos(ak_y)}{\tilde{E}_2^2} + \frac{\tilde{\epsilon} + 2J_{1b}\cos(ak_y)}{\tilde{E}_3^2} + \frac{\tilde{\epsilon} + 2J_{1b}\cos(ak_y)}{\tilde{E}_4^2} \right)} \quad (11)$$

3. NUMERICAL ANALYSIS AND DISCUSSION

In the previous section we have derived the analytical expression for the Neel temperature for the 122-type of pnictides within our bilayer model. From (11) we see that Neel temperature depends on model parameters namely its exchange integrals values and anisotropy. This section we will use to present numerical results on how Neel temperature depends on spin anisotropy and to present the transition temperature values for the wide range of model parameters values. We shall compare our results with experimentally available results for three 122-type pnictide compounds namely $CaFe_2As_2$, $BaFe_2As_2$ and $SrFe_2As_2$. We will show how does transition temperature depend on the set of parameters J_{1a}, J_{1b}, J_2, J_c, J_p and spin anisotropy given by η. For that purpose, we define dimensionless parameters $d = \frac{J_2}{J_{1a}}$, $b = \frac{J_{1b}}{J_{1a}}$, $c = \frac{J_c}{J_{1a}}$, $p = \frac{J_p}{J_{1a}}$ since the J_{1a} can be taken as the strongest one [16]. Figure 3 shows dependence of Neel temperature on spin anisotropy parameter η for the following selection of model parameters: J_{1a}=50.0 meV, d=0.6, c=0.02, b=-0.2, p=0.001. Results are presented for spin values S=1 and S=1/2.

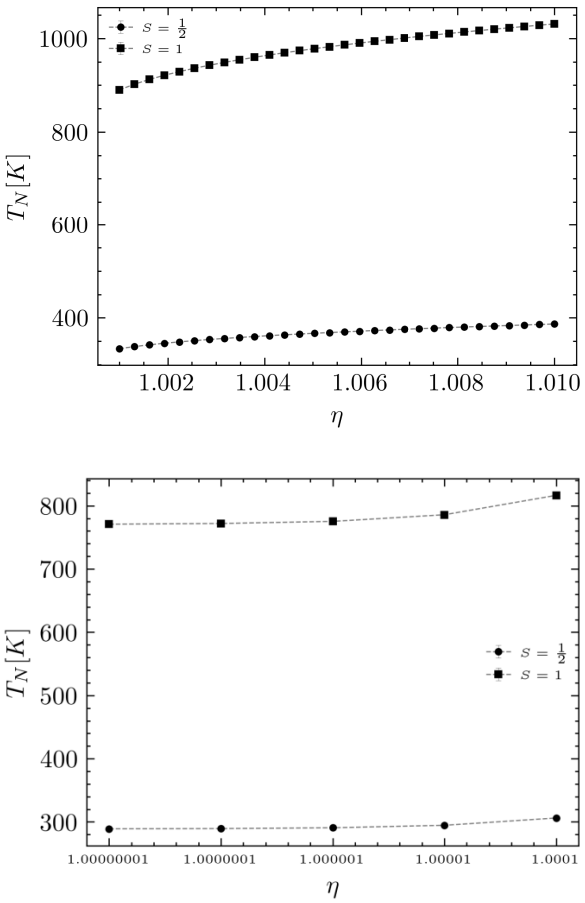

Figure 3. *The transition temperature dependence on the spin anisotropy parameter for spin values S=1/2 and S=1*

As can be seen from two parts of Figure 3, Neel temperature is an increasing function of the spin anisotropy parameter η, but with little change for value of η close to 1.0. Furthermore, we examine dependence of transition temperature on other model parameters b, c, d, p and J_{1a} at some value of spin anisotropy. In other words we investigate how does Neel temperature depend on exchange integrals J_{1a}, J_{1b}, J_2, J_c, J_p. Figure 4 shows dependence of transition temperature on the model exchange integrals.

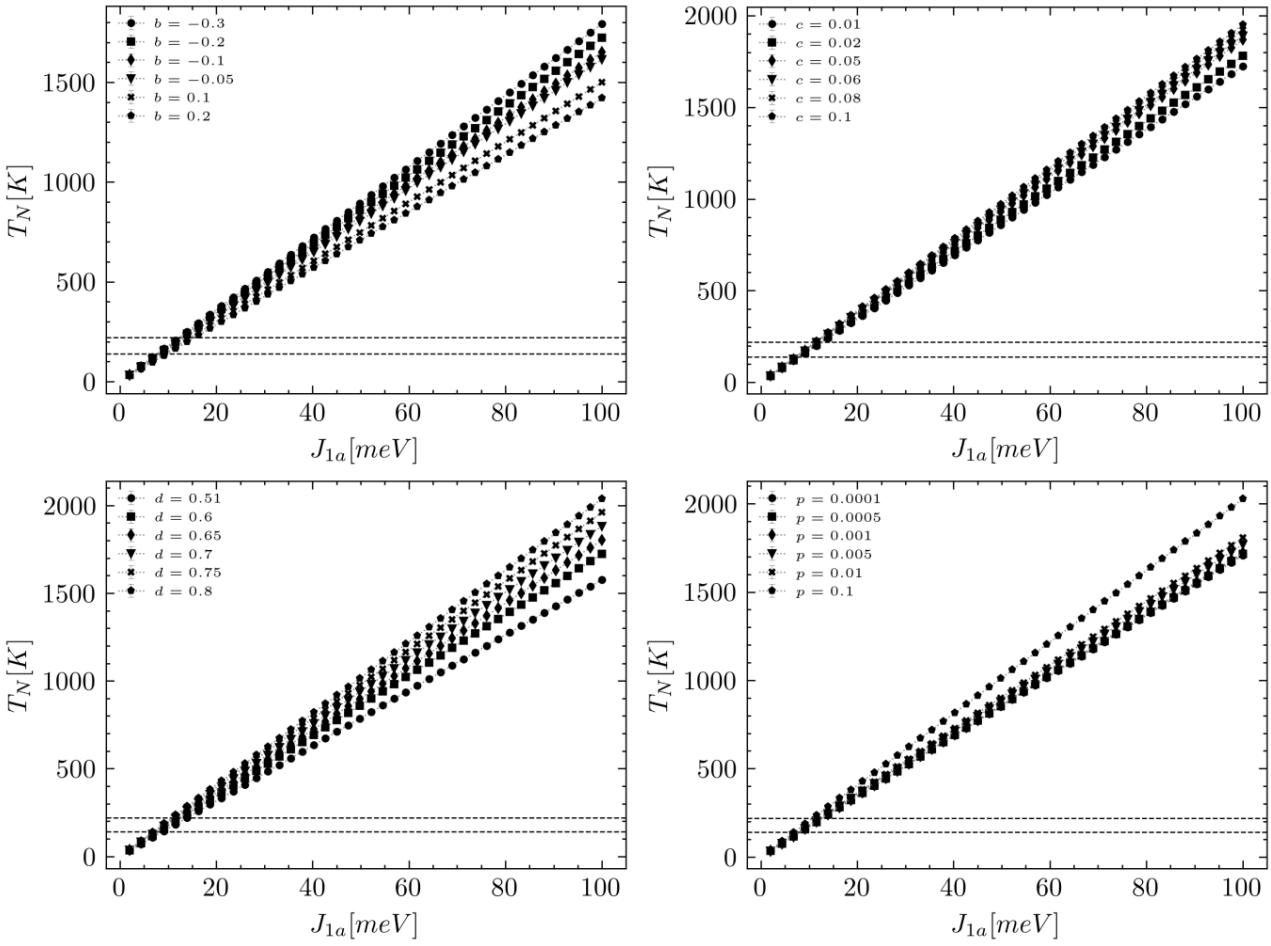

Figure 4. *Dependence of Neel temperature on J_{1a} for η=1.001 and (top left) c=0.01, d=0.6, p=0.001 and b=-0.3, -0.2,-0.1,-0.05,0.1,0.2, (top right) b=-0.2, d=0.6, p=0.001 and c=0.01,0.02,0.05,0.06,0.08,0.1, (bottom left) b= -0.2, c=0.01, p=0.001 and d=0.51,0.6,0.65,0.7,0.75,0.8 (bottom right) b=-0.2, c=0.01, d=0.6 and p=0.0001,0.0005,0.001,0.005,0.0, 0.1. All these results are for S=1*

From Figure 4 we see that that critical temperature grows with the increase of J_{1a} and other exchange integrals values. Two dashed horizontal lines in every part of Figure 4 cut the interval of Neel temperature values from 140 K to 220 K in which are the experimentally observed critical temperatures of $BaFe_2As_2$, $SrFe_2As_2$ and $CaFe_2As_2$ [11]. It is obvious that critical temperatures in that interval can be obtained for small values of J_{1a} and other corresponding parameters within our model. If we take S=1/2 those values will be higher. On the other hand, if we use parameters from other papers, the transition temperatures that we obtain are higher (>220 K) than the experimental measured values [14-17,24-28]. Finally, we examine the Neel temperature dependence on spin anisotropy for a range of J_{1a} values.

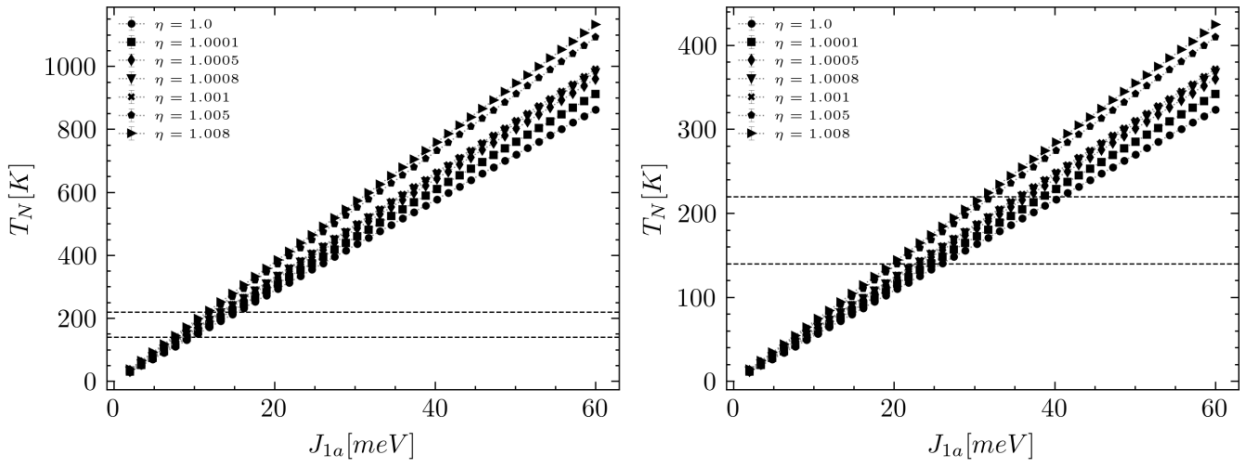

***Figure 5**. Transition temperature as a function of exchange integral J_{1a} for different values of η and b=-0.1, c=0.01, d=0.6, p=0.001: (left) S=1, (right) S=1/2*

If we look at Figure 5 we can once again conclude that Neel temperature grows with the increase of J_{1a} and η. Dashed horizontal lines correspond to already mentioned temperature interval. However, for the spin S=1/2 there is a shift to higher values of J_{1a} available to reproduce the Neel temperature of three mentioned 122-type compounds. With this we conclude the overview of our numerical results.

4. CONCLUSION

In this paper, we have derived transition temperature of the antiferromagnetic 122-type of iron pnictides based on the effective J_{1a}-J_{1b}-J_2-J_c-J_p Heisenberg model on a bilayer with anisotropy and for arbitrary spin. All the necessary calculations were done by using Green's functions method within the random phase approximation. Numerical calculations were done by using the analytical expression for the transition temperature in order to compare our results with some available data for the 122-type of iron pnictides. Our results suggest that spin anisotropy plays an important role in the magnetic properties of these compounds. We have given numerical results that are a map of sorts of the parameter space of available and possible magnetic interactions. In addition, overestimates of Neel temperature for parameters available in other papers might suggest that itinerant magnetism might play some important role in completely understanding the physical properties of iron pnictides. Results of our analysis should, with the rest available data, be helpful in better understanding the properties of 122-type of iron pnictide materials.

5. ACKNOWLEDGMENT

This work was supported by the Ministry of Education, Science and Technological Development of the Republic of Serbia (Grant No. 451-03-68/2020-14/200125 and Grant No. 451-03-68/2022-14/200122).

6. REFERENCES

[1] Y. Kamihara, T. Watanabe, M. Hirano, H. Hosono, Iron-based layered superconductor La[$O_{1-x}F_x$]FeAs (x= 0.05-0.12) with T_c=26 K, Journal of the American Chemical Society, Vol. 130-11 (2008) 3296-3297

[2] P. D. Johnson, G. Xu, W.-G. Yin (Eds.), Iron-based superconductivity, Springer Cham, Switzerland 2015, 3-112

[3] F. Mancini, R. Citro (Eds.), The iron pnictide superconductors: an introduction and overview, Springer Cham, Switzerland 2017, 1-6

[4] C. Wang, L. Li, S. Chi, Z. Zhu, Z. Ren, Y. Li, Y. Wang, X . Lin, Y. Luo, S. Jiang, X. Xu, G. Cao, Z. Xu, Thorium-doping-induced superconductivity up to 56 K in $Gd_{1-x}Th_xFeAsO$, Europhysics Letters, Vol. 83-6 (2008) 67006 (4pp)

[5] M. Rotter, M. Tegel, D. Johrendt, Superconductivity at 38 K in the iron arsenide ($Ba_{1-x}K_x$)

Fe_2As_2, Physical Review Letters, Vol. 101-10 (2008) 1007006 (4pp)

[6] C. W. Chu, F. Chen, M. Gooch, A. M. Guloy, B. Lorenz, B. Lv, K. Sasmal, Z. J. Tang, J. H. Tapp, Y. Y. Xue, The synthesis and characterization of LiFeAs and NaFeAs, Physica C: Superconductivity, Vol. 469-9 (2009) 326-331

[7] K.-W. Yeh, T.-W. Huang, Y.-L. Huang, T.-K. Chen, F.-C. Hsu, P. M. Wu, Y.-C. Lee, Y.-Y. Chu, C.-L. Chen, J.-Y. Luo, D.-C. Yan, M.-K. Wu, Tellurium substitution effect on superconductivity of the α-phase iron selenide, Europhysics Letters, Vol. 84-3 (2008) 37002 (4pp)

[8] A. Iyo, K. Kawashima, T. Kinjo, T. Nishio, S. Ishida, H. Fujihisa, Y. Gotoh, K. Kihou, H. Eisaki, Y. Yoshida, New-structure-type Fe-based superconductors: $CaAFe_4As_4$ (A=K, Rb, Cs) and $SrAFe_4As_4$ (A=Rb, Cs), Journal of the American Chemical Society, Vol. 138-10 (2016) 3410-3415

[9] X. Lu, D. D. Scherer, D. W. Tam, W. Zhang, R. Zhang, H. Luo, L. W. Harriger, H. C. Walker, D. T. Adroja, B. M. Andersen, P. Dai, Spin waves in detwinned $BaFe_2As_2$, Physical Review Letters, Vol. 121-6 (2018) 067002 (6pp)

[10] N. Plakida, High-temperature cuprate superconductors: experiment, theory and applications, Springer, Berlin 2010, 1-120

[11] M. D. Lumsden, A. D. Christianson, Magnetism in Fe-based superconductors, Journal of Physics: Condensed Matter, Vol. 22-20 (2010) 203203 (26pp)

[12] P. Dai, Antiferromagnetic order and spin dynamics in iron-based superconductors, Reviews of Modern Physics, Vol. 87-3 (2015) 855-896

[13] M. Vujinović, M. Pantić, D. Kapor, P. Mali, Theoretical models for magnetic properties of iron pnictides, International Journal of Modern Physics B, Vol. 27-16 (2013) 1350071 (18pp)

[14] J. Zhao, D.-X. Yao, S. Li, T. Hong, Y. Chen, S. Chang, W. Ratcliff II, J. W. Lynn, H. A. Mook, G. F. Chen, J. L. Luo, N. L. Wang, E. W. Carlson, J. Hu, P. Dai, Low energy spin waves and magnetic interactions in $SrFe_2As_2$, Physical Review Letters, Vol. 101-16 (2008) 167203 (4pp)

[15] J. Zhao, D. T. Adroja, D.-X. Yao, R. Bewley, S. Li, X. F. Wang, G. Wu, X. H. Chen, J. Hu, P. Dai, Spin waves and magnetic exchange interactions in $CaFe_2As_2$, Nature Physics, Vol. 5-8 (2009) 555-560

[16] R. Applegate, J. Oitmaa, R. R. P. Singh, Spin waves in J_{1a}-J_{1b}-J_2 orthorhombic square-lattice Heisenberg models: application to iron pnictide materials, Physical Review B, Vol. 81-2 (2010) 024505 (8pp)

[17] L. W. Harriger, H. Q. Luo, M. S. Liu, C. Frost, J. P. Hu, M. R. Norman, P. Dai, Nematic spin fluid in the tetragonal phase of $BaFe_2As_2$, Physical Review B, Vol. 84-5 (2011) 054544 (13pp)

[18] M. Pavkov, M. Škrinjar, D. Kapor, M. Pantić, S. Stojanović, Magnetic properties of antiferromagnetic bilayers analyzed in the spin and boson pictures, Physical Review B, Vol. 65-10 (2002) 104512 (8pp)

[19] M. Pantić, M. Škrinjar, D. Kapor, The analytical treatment of magnetic properties of three-layer ferrimagnetic superlattice, Physica A: Statistical Mechanics and its Applications, Vol. 387-23 (2008) 5786-5794

[20] W. Nolting, A. Ramakanth, Quantum theory of magnetism, Springer, Berlin 2009, 175-386

[21] M. Pantić, M. Rutonjski, P. Mali, M. Pavkov Hrvojević, S. Radošević, Anisotropy influence on the striped antiferromagnetism of a frustrated Heisenberg model: an application to iron pnictide materials, Contemporary Materials, Vol. 7-2 (2016) 121-136

[22] Y. Su, P. Link, A. Schneidewind, T. Wolf, P. Adelmann, Y. Xiao, M. Meven, R. Mittal, M. Rotter, D. Johrendt, T. Brueckel, M. Loewenhaupt, Antiferromagnetic ordering and structural phase transition in $BaFe_2As_2$ with Sn incorporated from growth flux, Physical Review B, Vol. 79-6 (2009) 064504 (6pp)

[23] S. V. Tyablikov, Methods in the Quantum Theory of Magnetism, Springer, New York 1967, 205-311

[24] K. Matan, R. Morinaga, K. Iida, T. J. Sato, Anisotropic itinerant magnetism and spin fluctuations in $BaFe_2As_2$: a neutron scattering study, Physical Review B, Vol. 79-5 (2009) 054526 (7pp)

[25] A. A. Aczel, E. Baggio-Saitovitch, S. L. Budko, P. C. Canfield, J. P. Carlo, G. F. Chen, P. Dai, T. Goko, W. Z. Hu, G. M. Luke, J. L. Luo, N. Ni, D. R. Sanchez-Candela, F. F. Tafti, N. L. Wang, T. J. Williams, W. Yu, Y. J. Uemura, Muon-spin-relaxation studies of magnetic order and superfluid density in antiferromagnetic NdFeAsO, $BaFe_2As_2$ and superconducting $Ba_{1-x}K_xFe_2As_2$, Physical Review B, Vol. 78-21 (2008) 214503 (5pp)

[26] Q. Huang, Y. Qiu, W. Bao, M. A. Green, J. W. Lynn, Y.C. Gasparovic, T. Wu, G. Wu, X. H. Chen, Neutron-diffraction measurements of magnetic order and a structural transition in the parent $BaFe_2As_2$ compound of FeAs-based high-temperature superconductors, Physical Review Letters, Vol. 101-25 (2008) 257003 (4pp)

[27] R. J. McQueeney, S. O. Diallo, V. P. Antropov, G. D. Samolyuk, C. Broholm, N. Ni, S. Nandi, M. Yethiraj, J. L. Zarestky, J. J. Pulikkotil, A. Kreyssig, M. D. Lumsden, B. N. Harmon, P. C. Canfield, A. I. Goldman, Anisotropic three-dimensional magnetism in $CaFe_2As_2$, Physical Review Letters, Vol. 101-22 (2008) 227205 (4pp)

[28] S. O. Diallo, V. P. Antropov, T. G. Perring, C. Broholm, J. J. Pulikkotil, N. Ni, S. L. Bud'ko, P. C. Canfield, A. Kreyssig, A. I. Goldman, R. J. McQueeney, Itinerant magnetic excitations in antiferromagnetic $CaFe_2As_2$, Physical Review Letters, Vol. 102-18 (2009) 187206 (4pp)

ЗАВИСНОСТ ПРЕЛАЗНЕ ТЕМПЕРАТУРЕ ОД АНИЗОТРОПИЈЕ У J_1-J_2-J_c-J_p ХАЈЗЕНБЕРГОВОМ МОДЕЛУ СА ПРИМЈЕНОМ НА 122 ТИП ПНИКТИДА НА БАЗИ ГВОЖЂА

Сажетак: У претходном периоду показано је значајно интересовање за проучавање суперпроводника на бази гвожђа названих пниктидима. Циљ овог рада је да допринесе бољем разумевању магнетних особина 122 класе пниктида гвожђа. Користимо анизотропни J_1-J_2-J_c-J_p Хајзенбергов модел. Коришћен је метод спинских Гринових функција у Тјабликовљевој апроксимацији случајних фаза како бисмо одредили израз за критичну температуру. На основу добијеног израза за критичну температуру разматрамо њену зависност од спинске анизотропије. Поред тога, упоређујемо резултате нашег модела са експериментално доступним подацима о критичној температури. Додатно, разматрамо вредности критичне температуре добијене нашим моделом користећи интеракције измене из других радова. Резултати које смо представили овде требало би да дају допринос разумевању магнетних особина 122 класе суперпроводника на бази гвожђа.

Кључне речи: Нелова температура, спинска анизотропија, пниктиди гвожђа, анизотропни Хајзенбергов модел.

Paper received: 29 August 2022 **Paper accepted: 10 November 2022**