Temperature-dependent striped antiferromagnetism of LaFeAsO in a Green’s function approach

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Received 10 February 2009, in final form 30 March 2009
Published 22 April 2009
Online at stacks.iop.org/JPhysCM/21/195701

Abstract
We use a Green’s function method to study the temperature-dependent average moment and magnetic phase-transition temperature of the striped antiferromagnetism of LaFeAsO, and other similar compounds, as the parents of FeAs-based superconductors. We consider the nearest and the next-nearest couplings in the FeAs layer, and the nearest coupling for inter-layer spin interaction. The dependence of the transition temperature $T_N$ and the zero-temperature average spin on the interaction constants is investigated. We obtain an analytical expression for $T_N$ and determine our temperature-dependent average spin from zero temperature to $T_N$ in terms of unified self-consistent equations. For LaFeAsO, we obtain a reasonable estimation of the coupling interactions with the experimental transition temperature $T_N = 138$ K. Our results also show that a non-zero antiferromagnetic (AFM) inter-layer coupling is essential for the existence of a non-zero $T_N$, and the many-body AFM fluctuations reduce substantially the low-temperature magnetic moment per Fe towards the experimental value. Our Green’s function approach can be used for other FeAs-based parent compounds and these results should be useful to understand the physical properties of FeAs-based superconductors.

(Some figures in this article are in colour only in the electronic version)

1. Introduction
The discovery of the high-temperature superconductor La$_{1-x}$Fe$_x$AsO$_{1+y}$ by Kamihara et al [1] has triggered worldwide research on all aspects of FeAs-based pnictides superconductors and their parent compounds, namely LnFeAsO ($Ln = La$ [1–7], Ce [8, 9], Pr [10], Nd [11, 12], Sm [13–15], …) and AF$_2$As$_2$ ($A = Ca$ [16–18], Sr [19–21], Ba [22, 23, 21]). LnFeAsO and AF$_2$As$_2$ have some common characteristics: (a) they are all of layered structure and have structure transitions from high-temperature tetragonal to low-temperature orthorhombic symmetry; (b) they all have stripe-like antiferromagnetic (AFM) order formed by Fe atoms, and the AFM transition temperatures $T_N$s are not higher than the structure transition temperatures $T_S$s; (c) the onset of superconductivity competes with the AFM and structure transitions [24, 25], and they differ in the sense that $T_N < T_S$ for LnFeAsO and $T_N = T_S$ for AF$_2$As$_2$. Both of the two series can be made superconducting by doping them with appropriate dopants or applying pressures. It should help in understanding the superconductivity of FeAs-based materials to elucidate the corresponding antiferromagnetism of the parent compounds.

LaFeAsO is the prototype and the representative of the parent compounds of FeAs-based superconductors, and thus we focus on the striped AFM order of undoped LaFeAsO, whose $T_N$ is 138 K and $T_S$ 156 K [2, 3]. First-principles results confirm that the stripe-AFM order is the magnetic ground state [5]. Spin-wave approaches were adopted to give the low-temperature excitation spectra [7, 26, 19], and the spin–orbit interaction and p–d hybridization are used to explain the
observed small magnetic moment $0.25 \mu_B \sim 0.36 \mu_B$ per Fe at low temperature [2, 3, 6]. However, it is highly desirable to describe the magnetic moment from zero temperature to $T_N$ within a unified theory.

In this paper, we use a Green’s function method to study the temperature-dependent average moment and phase-transition temperature of the striped antiferromagnetism of LaFeAsO, and other similar compounds, as the parents of FeAs-based superconductors. We consider the nearest and the next-nearest couplings in the FeAs layer, and only the nearest one for the inter-layer spin interaction. The dependence of the transition temperature $T_N$ and the zero-temperature average spin on the four interactions are investigated. We obtain an analytical expression for $T_N$, and determine our temperature-dependent average spin from zero temperature to $T_N$ in terms of unified self-consistent equations. For LaFeAsO, we obtain a reasonable estimation of the coupling interactions with experimental phase-transition temperature $T_N = 138$ K. Our results also show that a non-zero antiferromagnetic inter-layer coupling is essential for the existence of a non-zero $T_N$, and the many-body AFM fluctuations reduce substantially the low-temperature magnetic moment per Fe towards the experimental value. More detailed results will be presented. The remaining part of this paper is organized as follows. In section 2, we shall give our spin model, the Green’s function derivation and our main analytical results. In section 3, we shall present our numerical results and make corresponding discussions. Our conclusion is given in section 4.

2. Effective model, Green’s function derivation, and main analytical results

To deal with the striped AFM configuration of LaFeAsO, we consider the Fe lattice of the original orthorhombic LaFeAsO structure and divide it into two sublattices, in each of which the Fe spins align parallel but are antiparallel between the two sublattices (figure 1). Hence we consider an anisotropic Heisenberg Hamiltonian

$$\hat{H} = \sum_{i,j} J_{i,j} \mathbf{S}_i \cdot \mathbf{S}_j + J_a \sum_{i,j} \mathbf{S}_i \cdot \mathbf{S}_j,$$

in which $\mathbf{S}_i$ denotes the quantum spin operator at the lattice position $i$, $(i, j)$ means nearest-neighbor (NN) spin pairs, and $\langle\langle i, j \rangle\rangle$ means next-nearest-neighbor (NNN) spin pairs in the $a-b$ plane (we only consider NNN pairs in the $a-b$ plane because the inter-layer interactions are very weak). The NN interaction $J_{i,j}$ can be three values: $J_{ia}$ which is the spin interaction between parallel NN spins in the $a-b$ plane, $J_{ib}$ between antiparallel NN spins in the $a-b$ plane and $J_c$ between the inter-layer NN spins. $J_2$ is the interaction between NNN spins in the $a-b$ plane. Four different $J$s make $\hat{H}$ anisotropic. To differentiate the spin operators in SL1 and SL2, we use $\mathbf{S}_{i1}$ and $\mathbf{S}_{j2}$ to represent them, respectively. For spins in SL2, we make transformations: $\mathbf{S}_{i2} = -\mathbf{S}_{i1}$, $\mathbf{S}_{j2} = \mathbf{S}_{j1}$, $\mathbf{S}^z_{i2} = \mathbf{S}^z_{i1}$ and then have

$$\mathbf{S}_{i1} \cdot \mathbf{S}_{j2} = \frac{1}{2} (\mathbf{S}^z_{i1} \mathbf{S}^z_{j2} + \mathbf{S}^z_{i1} \mathbf{S}^z_{j2}) + \mathbf{S}_{i1} \mathbf{S}_{j2}$$

Inserting (2) into (1) we can get the Hamiltonian expressed by $\mathbf{S}_{i1}$ and $\mathbf{S}_{j2}$ (simple but too long to give out here).

Accordingly, we use a Green’s function method [27, 28] to solve the model (1). In this scheme one uses a double-time Green’s function $\langle\langle \hat{A}(t); \hat{B}(t') \rangle\rangle$ ($\hat{A}$ and $\hat{B}$ represent two arbitrary quantum operators) which satisfies the following equation of motion:

$$i\hbar \frac{d}{dt}\langle\langle \hat{A}(t); \hat{B}(t') \rangle\rangle = \langle\langle \{\hat{A}(t), \hat{B}(t') \} \rangle\rangle$$

This approach proves successful for various Heisenberg spin models [27–32]. In [30], there is a detailed but somewhat long derivation about the Green’s function method for Heisenberg spin models, and by considering this derivation, we conclude that the process of using Green’s functions to solve the average spin of a Heisenberg model can be simplified into three steps: (a) construct Green’s functions $\langle\langle \hat{S}_{i1}^z; \hat{S}_{j2}^z \rangle\rangle$ and their equations of motion via (3) and then use a Tyablikov cutoff approximation (4) to decouple the equations of motion [28];

$$(\langle\langle \hat{S}_1^z; \hat{B}_j \rangle\rangle \mapsto \langle\langle \hat{S}_1^z; \hat{B}_j \rangle\rangle) \rightarrow \langle\langle \hat{S}_1^z; \hat{B}^\dagger \rangle\rangle$$

(b) use the spectrum theorem to express the correlation function $\langle\langle \hat{S}_1^z; \hat{B}^\dagger \rangle\rangle$ in term of the average spin $z$-component $\langle\langle \hat{S}_1^z \rangle\rangle$ and then obtain the $\Phi(\langle\langle \hat{S}_1^z \rangle\rangle)$ function

$$\Phi(\langle\langle \hat{S}_1^z \rangle\rangle) = \frac{1}{2} \langle\langle \hat{S}_1^z \rangle\rangle,$$

(c) use the Callen expression (6) [30] to evaluate $\langle\langle \hat{S}_1^z \rangle\rangle$ self-consistently

$$\langle\langle \hat{S}_1^z \rangle\rangle = \frac{(S - \Phi)(1 + \Phi)^{2S+1} + (S + 1 + \Phi)\Phi^{2S+1}}{(1 + \Phi)^{2S+1} - \Phi^{2S+1}}.$$  

According to the three steps given above, for our spin system we construct double-time spin Green’s functions between spin operators at two positions $i$ and $j$ in SL1

$$\bar{G}_{ij}^{(1)}(t, t') = \langle\langle \hat{S}_{i1}^z(t); \hat{S}_{j2}^z(t') \rangle\rangle$$
and Green’s functions between spin operators at two positions in SL2 and \( j' \) in SL1
\[
\hat{G}_{ij}^{(11)}(t, t') = \langle \hat{S}_i^{r}(t); \hat{S}_j^{r}(t') \rangle. \tag{8}
\]

Equation (7) can be expressed as a Fourier expansion
\[
\hat{G}_{ij}^{(11)}(t, t') = \frac{1}{2\pi h} \int G_{ij}^{(11)}(\omega)e^{-i\omega(t-t')/h} d\omega, \tag{9}
\]
because the Hamiltonian (1) is time independent, and (8) is similar. Assuming that each spin has the same average \( \langle \hat{S}_i^{r} \rangle \) for SL1 and \( \langle \hat{S}_i^{r} \rangle \) for SL2, and because of the AFM symmetry plus the transformation (2), we have \( \langle \hat{S}_i^{r} \rangle = \langle \hat{S}_i^{r} \rangle = \langle \hat{S}_i^{r} \rangle \). Then using the Fourier transformation as shown in (9), making the Tyablikov cutoff approximation to decouple the equations of motion, and another Fourier transformation from lattice sites real space to \( k \) space, we have
\[
1 + \mathcal{S}_k^{(1)} \left[ J_{1b} \rho_1(k) - \frac{\omega}{2} \langle \hat{S}_i^{r} \rangle \right] + J_{1b} \mathcal{S}_k^{(2)} \rho_2(k) = 0 \tag{10}
\]
and
\[
\mathcal{S}_k^{(1)} J_{1b} \rho_2(k) + \mathcal{S}_k^{(2)} \left[ J_{1b} \rho_1(k) + \frac{\omega}{2} \langle \hat{S}_i^{r} \rangle \right] = 0, \tag{11}
\]
in which
\[
\mathcal{S}_k^{(1)} = \sum_r G_{k+r}^{(11)}(\omega)e^{-i\mathbf{k}\cdot\mathbf{r}}, \tag{12}
\]
\[
\mathcal{S}_k^{(2)} = \sum_r G_{k+r}^{(2)}(\omega)e^{-i\mathbf{k}\cdot\mathbf{r}}, \tag{13}
\]
and
\[
\rho_1(k) = -p(1 - \cos \mathbf{k} \cdot \mathbf{a}) + 1 + 2q + r \tag{14}
\]
\[
\rho_2(k) = (1 + 2q \cos \mathbf{k} \cdot \mathbf{a}) \cos \mathbf{k} \cdot \mathbf{b} + r \cos \mathbf{k} \cdot \mathbf{c},
\]
where \( E(k) \) is the spin excitation spectrum defined by
\[
E(k) = 2J_{1b} \langle \hat{S}_i^{r} \rangle \sqrt{\rho_1^2(k) - \rho_2^2(k)}. \tag{15}
\]
And from \( \mathcal{S}_k^{(1)} \) we get
\[
G_{ij}^{(11)}(\omega) = \frac{1}{N} \sum_{k \in \text{BZ}} \mathcal{S}_k^{(1)} e^{i\mathbf{k}(i-j)} \tag{16}
\]
in which \( N \) is the total number of spins in SL1 and SL2, and \( \text{BZ} \) denotes the first Brillouin zone (there are \( N \) \( k \)-points in \( \text{BZ} \)). Using the spectrum theorem and letting \( j = i \), we get the correlation function \( \langle \hat{S}_i^{r} \rangle \langle \hat{S}_i^{r} \rangle \) as follow
\[
\langle \hat{S}_i^{r} \rangle \langle \hat{S}_i^{r} \rangle \rangle = -\frac{1}{\pi} \int_{-\infty}^{\infty} \operatorname{Im}[G_{ii}^{(11)}(\omega + i0^+)] e^{\beta\omega - 1} d\omega \tag{17}
\]
where \( \beta = 1/(k_B T) \), \( T \) is temperature, and \( k_B \) is the Boltzmann constant. Then using (5) we get the \( \Phi \) function:
\[
\Phi(\langle \hat{S}_i^{r} \rangle) = \frac{1}{2N} \sum_{k \in \text{BZ}} \frac{\rho_1}{\sqrt{\rho_1^2 - \rho_2^2}} \tag{18}
\]
Now, the average spin z-component \( \langle \hat{S}_i^{r} \rangle \) can be obtained easily by self-consistently solving (19) and (6). A special case is that when the temperature \( T = 0 \), \( \operatorname{coth} \frac{\beta \rho_1}{2} \rightarrow 1 \), and we have
\[
\Phi_0(\Phi|_{T=0}) = \frac{1}{2N} \sum_{k \in \text{BZ}} \frac{\rho_1}{\sqrt{\rho_1^2 - \rho_2^2}} \tag{19}
\]
At this time, \( \Phi_0 \) is no longer dependent on \( \langle \hat{S}_i^{r} \rangle \) and the zero-temperature average spin z-component \( \langle \hat{S}_i^{r} \rangle \rangle \) can be obtained directly by inserting (20) into (6).

While the temperature approaches \( T_N \), \( \langle \hat{S}_i^{r} \rangle \) approaches zero and, further, \( E(k) \rightarrow 0 \) and \( \Phi \rightarrow \infty \). Expanding (19) and (6), we derive
\[
\langle \hat{S}_i^{r} \rangle \ll \sqrt{1 - \frac{T}{T_N}}, \tag{20}
\]
where \( T_N \) is defined by
\[
T_N = \frac{2J_{1b} \langle \hat{S}_i^{r} \rangle(s + 1)}{3G k_B} \tag{21}
\]
and \( \Gamma = \frac{1}{N} \sum_k \rho_1/(\rho_1^2 - \rho_2^2) \).

3. Numerical results and discussions

There is no consensus on the magnitudes of the coupling interactions \( J_{1a}, J_{1b}, J_2, J_c \) in FeAs-based pnictides, and many authors only consider two or three of them \([4, 5, 33, 23, 19, 16, 34]\). Yildirim’s first-principles results show that \( J_1 \approx J_2 \). However, we prefer the opinion that \( J_{1a} = J_{1b} \). This could be mediated by two Fe–As–Fe paths (figure 2(a)) and this should mean \( J_{1a} \neq J_{1b} \), but in the small structural change from tetragonal to orthorhombic symmetry. \( J_2 \) is mediated by only one Fe–As–Fe path (figure 2(a)) and this should give \( J_2 \approx J_{1a} \). From the viewpoint of classical favorable energy in forming stripe-like
AFM patterns along the $\alpha$ direction, as shown in figure 2(b) (see figures 2(b)–(d) and (23)), we have,

$$E_{(b)} = 4J_{1a}S^2 - 4J_{1b}S^2 - 8J_2S^2$$
$$E_{(c)} = -4J_{1b}S^2 + 4J_{1b}S^2 - 8J_2S^2$$
$$E_{(d)} = -4J_{1b}S^2 - 4J_{1b}S^2 + 8J_2S^2.$$  \hspace{1cm} (23)

This should mean $J_{1a} < J_{1b}$ and $2J_2 > J_{1a}$, which in fact are just the conditions that fulfill $\rho_{12}^2 - \rho_{12}^2 \geq 0$ to make $E(k)$ in (16) meaningful. As for $J_c$, it is a very weak long-range AFM interaction whose origin is unclear except for the superexchange. Therefore, in terms of $p$, $q$, $r$ in (14), we confine the coupling interactions as follows:

$$1 \geq p \geq 1 - \delta_p$$
$$p/2 < q < p/2 + \delta_q,$$  \hspace{1cm} (24)

$$0 < r \leq \delta_r$$

where $\delta_p$, $\delta_q$, and $\delta_r$ are the confine parameters for $p$, $q$, and $r$, respectively, and they fulfill $0 < \delta_p, \delta_q, \delta_r \ll 1$. The lhs of (24) represents the necessary conditions for forming striped AFM ordering along the $\alpha$ direction, and the rhs the conditions for limiting $p$, $q$, and $r$ within small regions.

From figure 3 we can see that $T_N$ increases as $q$ and $r$ increase but decreases as $p$ increases. It is easy to understand. NNN spins and inter-layer NN spins all align antiparallel, so bigger AFM coupling interactions will lower the system’s energy, stabilize the AFM configuration and hence enhance $T_N$; in contrast, spins along the $\alpha$ direction align parallel but have AFM interactions, therefore a bigger $p$ will increase the system’s energy, destabilize the AFM configuration and hence decrease $T_N$. Note that while $q \to p/2$ or $r \to 0$, $T_N \to 0$, that is to say, both the existence of an AFM inter-layer interaction $J_c$ and the condition $2J_2 > J_{1a}$ are essential to form striped AFM ordering. In fact, when $r = 0$ this system becomes two-dimensional, and the result of $T_N = 0$ in two-dimensions is analogous to the Mermin–Wagner theorem for isotropic interactions [38]. We also see that the critical condition $p = 1$ does not lead to $T_N \to 0$, which shows that $J_{1a} = J_{1b}$ is not a fatal factor to kill $T_N$ but only a critical value to separate the two cases shown in figures 2(b) and (c).

The magnetic moment per Fe of LaFeAsO at low temperature is reported experimentally as 0.36 $\mu_B$ [2] or 0.25 $\mu_B$ [3], both of which are very small compared to the first-principles values 2.2–2.4 $\mu_B$/Fe [39, 40]. Accordingly, we choose $S = 1$ in our model (assuming the Landé $g$-factor equals 2). Figure 4 shows the zero-temperature average spin $\langle \hat{S}^z \rangle_0$. Similar to $T_N$, $\langle \hat{S}^z \rangle_0$ is also an increasing function...
of both \( q \) and \( r \) but a decreasing function of \( p \). However, \( \langle \hat{S}^z \rangle_0 \rightarrow 0 \) only when both \( r \rightarrow 0 \) and \( q \rightarrow p/2 \). When only \( r \rightarrow 0 \) or \( q \rightarrow p/2 \) is met, \( \langle \hat{S}^z \rangle_0 \) approaches a minimum but not zero, while at the same time \( T_N \rightarrow 0 \).

There are four \( J_s \) in our model. What are their values? Let us have a look at what they can be under the condition \( T_N = 138 \) K. Figure 5 shows the regions available for \( p, q \) and \( r \) under conditions (24), with \( \delta_p = 0.05, \delta_q = 0.05 \) and \( \delta_r = 0.001 \), in orange (gray) color for \( J_{1b} = 40 \) meV, 50 meV, and 60 meV, respectively. The smaller \( J_{1b} \), the smaller the parameter region available. Hence, for given \( \delta_p, \delta_q \) and \( \delta_r \), there is a lower limit for \( J_{1b} \) to fulfil a given \( T_N \). This lower limit, written as \( J_{1b}^{\text{min}} \), is given in table 1, which shows that the smaller each of \( \delta_p, \delta_q \) and \( \delta_r \) is, the bigger \( J_{1b}^{\text{min}} \) is. However, although no upper limit for \( J_{1b} \) is given, \( J_{1b} \) cannot be infinitely large. In fact, first-principles results show that \( J_{1b} \sim 50 \) meV [4, 33].

Here we did not use the experimental data for the low-temperature magnetic moment per Fe atom, which amounts to \( \langle \hat{S}^z \rangle_0 = 0.13–0.18 \), to determine the \( J_s \), because it is too small. If \( \langle \hat{S}^z \rangle_0 = 0.18 \) is met, we must have \( \delta_r < 10^{-6} \), even if \( q = p/2 \) is taken to minimize \( \langle \hat{S}^z \rangle_0 \) (see inset of figure 4). Such a tiny \( r \) definitely cannot fall within the orange (gray) area in figure 5 with a reasonable \( J_{1b} \) to fulfil \( T_N = 138 \) K. That is to say, although the many-body AFM fluctuations substantially reduce the low-temperature magnetic moment per Fe, they cannot be in full charge of the very small low-temperature magnetic moment which indeed is also ascribed to spin–orbit and \( p-d \) hybridization etc [6].

We choose three sets of \( J_s \) from the regions available in figure 5 for estimation (the three stars): \( \langle p, q, r \rangle = (0.955, 0.526, 0.0009), (0.98, 0.53, 0.0003) \), and \( (0.99, 0.53, 0.0001) \), for \( J_{1b} = 40 \) meV, 50 meV, and 60 meV, respectively. In terms of \( J_{1b}, J_{1a}, J_2 \) and \( J_c \), we can refer to them as \( J_{1b} = 50 \pm 10 \) meV, \( J_{1a} = 49 \pm 10 \) meV, \( J_2 = 26 \pm 5 \) meV, and \( J_c = 0.020 \pm 0.015 \) meV. The average spin \( \langle \hat{S}^z \rangle \) versus temperature \( T \) curves with the three sets of parameters given above are shown in figure 6.

We take LaFeAsO as an example here, however our calculations are not restricted to LaFeAsO, because nearly all LnFeAsO have similar or even the same transition temperatures (see table 2). It seems that \( T_N \) does not vary much with different Ln. This is in contrast to \( \text{AF}_2\text{As}_2 \), whose \( T_N \) varies with \( A: T_N = 172.5 \) K [18] for \( A = \text{Ca} \); \( T_N = 198 \) K [20], 205 K [42] or 220 K [43] for \( A = \text{Sr} \) and \( T_N = 140 \) K [22] or 135 K [44] for \( A = \text{Ba} \). Although there are some differences of structure between LnFeAsO and \( \text{AF}_2\text{As}_2 \),
we believe that our model works well for both of them, because they both have layered structures with stripe-like AFM order formed by Fe atoms. Indeed, this can also be extended to Fe(SeTe) [45, 46], which has nearly the same properties and can be superconducting under certain conditions.

4. Conclusion

In summary, we use a Green’s function method to study the striped AFM order formed by Fe atoms in LnFeAsO which is a representative of the parent compounds of recently discovered Fe-based superconductors. We take LaFeAsO as the example to analyze the AFM transition temperature \( T_N \) and zero-temperature average spin \( \langle \hat{S} \rangle_0 \), and show that both \( T_N \) and \( \langle \hat{S} \rangle_0 \) are increasing functions of \( J_{1b} \), \( J_2 \) and \( J_b \) but decreasing functions of \( J_{1a} \). By using \( T_N = 138 \, K \), we make a reasonable estimation of the coupling interactions, \( J_{1b} = 50 \pm 10 \, meV \), \( J_{1a} = 49 \pm 10 \, meV \), \( J_2 = 26 \pm 5 \, meV \), and \( J_b = 0.020 \pm 0.015 \, meV \). The average spin \( \langle \hat{S} \rangle \) is determined in the same way from zero temperature to \( T_N \), and \( T_N \) is expressed analytically. Our results also show that a non-zero AFM inter-layer coupling \( J_b \) is essential for the existence of a non-zero \( T_N \) and that the AFM fluctuations substantially reduce the low-temperature magnetic moment towards the small experimental value. Although our results cannot determine the relations between structure and AFM transitions, we believe that the AFM transition is most likely caused by the structure transition, because most of the experimental results show \( T_N \leq T_S \) for FeAs-based pnictides. Our Green’s function approach to the striped AFM properties can be used for other FeAs-based parent compounds.

Acknowledgments

This work is supported by the Nature Science Foundation of China (Grant Nos 10874232 and 10774180), by the Chinese Academy of Sciences (Grant No. KJCX2.YW.W09-5), and by the Chinese Department of Science and Technology (Grant No. 2005CB623602).

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