Role of Three Bands on Coexistence of Superconductivity and Antiferromagnetism in Samarium Iron Pnictide Superconductor

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Abstract

The coexistence of long range magnetic order and superconductivity in the iron pnictide superconductor SmFeAsO$_{1-x}$F$_x$ is the basis for the present study that analyses theoretically the role of multiple bands on the coexistence of superconductivity (SC) and antiferromagnetism (AFM). For this, a model Hamiltonian is developed and using Green’s function technique, expressions for $T_C$, $T_M$ and magnetic order parameter $\eta$ are obtained. For one band, two band and three band models separately, variation of $T_C$, $T_M$ with $\eta$ is studied. Further, the coexistence region has been extracted using the above information. The results show that superconducting and AFM order can coexist in this class of superconductors and increasing the number of bands increases the coexistence region.

Subject Areas

Condensed State Physics

Keywords

Superconductivity, Antiferromagnetism, Superconducting Order Parameter, Magnetic Order Parameter

1. Introduction

The iron pnictide superconductors [1] [2] [3] provide promising avenue for research as a lot many features set them apart from known superconductors along with the hitherto high $T_C$ found in this class of superconductors.

Iron pnictides stand second in line after the cuprates [4] to show high $T_C$ of around 55 K [5]. These transition metal based superconductors of the 1111 fam-
ily having general formula LnOFeAs (Ln = La, Ce, Sm, Gd, Nd, Pr) are layered structures with alternate LnO & FeAs layers, superconductivity believed to be present in the FeAs layers [6]. The atomic structure [7] of the 1111 family consists of negatively charged FeP or FeAs layers, where Fe atoms form a planar square lattice, and positively charged LnO layers, The structure orientation of Fe atoms shows it to be surrounded by four arsenic atoms resulting in a distorted tetrahedral geometry. The iron atoms are seen to make a square lattice and arsenic atoms are placed at the centre of each square being displaced above & below the Fe planes. It has been shown that in the normal state, these compounds are semi-metals [8] (upon doping [9] or application of pressure [10] [11] [12] [13] is seen to increase $T_C$ in iron pnictides). Angle resolved photoemission experiments [14] have demonstrated that iron pnictides are multiband [15] [16] in nature. Iron has five bands at the Fermi surface and all the five d-bands of iron are relevant in studying the superconducting properties of these compounds. Previous theories have found that multiband nature [17] of iron pnictides makes them a significant class in the vast area of superconductivity and that multiband superconductivity serves as an important ingredient for high $T_C$ for this class of compounds. The four unpaired d electrons of iron are seen to hybridise [18] with the three unpaired p electrons of arsenic, resulting in bands found at the Fermi surface due to overlapping orbitals [19] [20]. Raghu [21] et al. has discussed a minimal two band model [22] [23] is needed for the superconducting iron pnictides. Two band BCS superconductivity is studied by Maksimov [24] et al. for the compound Ba(Fe$_{0.9}$CO$_{0.1}$)$_2$As$_2$. Three band superconductivity [25] [26] [27] is also studied and Ummarino [28] has suggested that a simple three band model in strong-coupling regime can reproduce in a quantitative way the experimental $T_C$. Thus the multiband property of these compounds helps in better understanding of these materials.

Another feature that has created a lot of interest among researchers is the coexistence of superconductivity and magnetism [29] [30] [31] [32] in these superconductors. Extensive experimentation is carried out in various compounds [33] that has shown both the superconducting order parameter and the magnetic order parameter to coexist [34] [35] simultaneously. Theoretical study based on single band model [36] has been carried by Abera Mebrahtu et al. showing coexistence of superconductivity and AFM in SmAsO$_{1-x}$F$_x$Fe. Also the interplay of superconductivity and magnetism in FeAs based superconductors is studied theoretically [37] by Mesfin A. Afrassa et al. Some other theoretical studies include coexistence of superconductivity and spin density wave in ferropnictide Ba$_{1-x}$K$_x$Fe$_2$As$_2$ [38], the coexistence of superconductivity and ferromagnetism [39] and coexistence of superconducting and magnetic order in one band and two band SmOFeAs superconductor [40].

In view of the above, the present theoretical work aims to explore the role of multiband SmOFeAs superconductor. In this work, using Green’s function technique [41], we have studied coexistence of the two orders for one band, two band and three band models and to understand the behaviour of the two orders
existing simultaneously. Expressions for $T_C$, $T_M$ and $\eta$ are obtained as a function of the number of bands and the coexistence region is extracted from them.

### 2. Theoretical Model System Hamiltonian

The model Hamiltonian for study of magnetic properties using both localized and itinerant nature of electrons is written as:

$$
H = \sum_{m\sigma} E_{m\sigma} a_{m\sigma}^\dagger a_{m\sigma} + \sum_{\rho\sigma} E_{\rho\sigma} b_{\rho\sigma}^\dagger b_{\rho\sigma} - \sum_{m\sigma}\sum_{m'\sigma'} V_{BCS} a_{m\sigma}^\dagger a_{m\sigma'}^\dagger \sum_{\rho\sigma} \sum_{m'\sigma'} V_{\rho\sigma} a_{\rho\sigma}^\dagger a_{m'\sigma'}^\dagger a_{m'\sigma'} \frac{\Delta_{m'\sigma'}}{\Delta_{m\sigma}} + \sum_{m\sigma} \frac{\Delta_{m\sigma}}{\Delta_{m\sigma}} \sum_{\rho\sigma} \sum_{m'\sigma'} V_{\rho\sigma} a_{\rho\sigma}^\dagger a_{m'\sigma'}^\dagger a_{m'\sigma'} \frac{\Delta_{m'\sigma'}}{\Delta_{m\sigma}}$$

The first term represents energy of itinerant electrons. The second term denotes energy of localised electrons. The third term is the interaction between electron and electron through boson (phonon). The fourth term is the interaction term between conduction electrons and localized electrons due to some unspecified mechanism with coupling constant $\alpha$. The fifth term represents interband interaction.

Here $m$, $n$ are the band indices, $k$ is wave vector, $\sigma$ is spin of fermions and $p$ is site index for localized electrons. Operator ‘$a$’ is for conduction electrons and operator ‘$b$’ is for localized electrons.

### Coexistence of Superconductivity and Antiferromagnetism

In this section, magnetic properties of magnetic order parameter and coexistence of superconductivity and magnetism is investigated as a function of the number of bands using Green’s function formalism.

Considering the two Green’s functions for conduction electrons:

$$
G_{\uparrow\uparrow}^{\tau\tau} = \{\{a_{\downarrow\uparrow}^\dagger, a_{\uparrow\downarrow}^\dagger\}\} \quad (2a)
$$

$$
G_{\downarrow\uparrow}^{\tau\tau} = \{\{a_{\uparrow\downarrow}^\dagger, a_{\downarrow\uparrow}^\dagger\}\} \quad (2b)
$$

Following two equations of motion are obtained:

$$
\omega - E_{\downarrow\uparrow}^\dagger + V_{BCS} \gamma_{\downarrow\uparrow} G_{\uparrow\uparrow}^{\tau\tau} = \frac{\delta_{\tau\tau}}{2\pi} \left[ \Delta_{\tau\tau} + \sum_{\rho\sigma} \Delta_{\rho\sigma} - n_{\tau\tau} \right] G_{\rho\sigma}^{\tau\tau} - \sum_{\rho\sigma} \gamma_{\rho\sigma}^\downarrow G_{\rho\sigma}^{\tau\tau} + \sum_{\rho\sigma} V_{\rho\sigma} G_{\rho\sigma}^{\tau\tau} + \sum_{\rho\sigma} V_{\rho\sigma} \gamma_{\rho\sigma}^\downarrow G_{\rho\sigma}^{\tau\tau} + \sum_{\rho\sigma} V_{\rho\sigma} \gamma_{\rho\sigma}^\downarrow G_{\rho\sigma}^{\tau\tau} \quad (3)
$$

$$
\omega + E_{\downarrow\uparrow}^\dagger - V_{BCS} \gamma_{\downarrow\uparrow} G_{\downarrow\uparrow}^{\tau\tau} = - \left[ \Delta_{\tau\tau} + \sum_{\rho\sigma} \Delta_{\rho\sigma} - n_{\tau\tau} \right] G_{\rho\sigma}^{\tau\tau} + \sum_{\rho\sigma} \gamma_{\rho\sigma}^\uparrow G_{\rho\sigma}^{\tau\tau} + \sum_{\rho\sigma} V_{\rho\sigma} G_{\rho\sigma}^{\tau\tau} + \sum_{\rho\sigma} V_{\rho\sigma} \gamma_{\rho\sigma}^\uparrow G_{\rho\sigma}^{\tau\tau} + \sum_{\rho\sigma} V_{\rho\sigma} \gamma_{\rho\sigma}^\uparrow G_{\rho\sigma}^{\tau\tau} \quad (4)
$$

In the calculations that follow, the following Green’s functions are used:

$$
G_i = G_{\tau\tau}^{\tau\tau} \quad (11q) \quad (3)
$$

$$
G_2 = G_{\downarrow\uparrow}^{\tau\tau} \quad (11q) \quad (4)
$$
Solving for one band model

The superconducting order parameter is defined as:

$$\Delta_{11} = \sum_k V_{11} \langle a_{11 \uparrow}, a_{11 \downarrow} \rangle$$

The correlation function is obtained as:

$$\langle a_{1k \uparrow}, a_{1k \downarrow} \rangle = -\frac{1}{i} \int_{-\infty}^{\infty} \frac{G_z(\omega + i\varepsilon) - G_z(\omega - i\varepsilon)}{e^{\frac{\omega}{kT}} - \eta} d\omega$$

$$= \frac{\Delta_{11} - \eta_1}{2} \tanh \left( \frac{\sqrt{(E_{1q \uparrow} - V_{BCS} \gamma)^2 + (\Delta_{11} - \eta_1)^2}}{2kT} \right)$$

$$\text{(5)}$$

Solving for two band model

The first correlation function is obtained as:

$$\langle a_{1k \uparrow}, a_{1k \downarrow} \rangle$$

$$= \frac{V_{12} \Delta_{22} + \Delta_{11} - \eta_1}{2} \tanh \left( \frac{\sqrt{(E_{1q \uparrow} - V_{BCS} \gamma)^2 + (\Delta_{11} - \eta_1)^2}}{2kT} \right)$$

$$\text{(6)}$$

The second correlation function is written as:

$$\langle a_{2k \uparrow}, a_{2k \downarrow} \rangle = -\frac{1}{i} \int_{-\infty}^{\infty} \frac{G_b(\omega + i\varepsilon) - G_b(\omega - i\varepsilon)}{e^{\frac{\omega}{kT}} - \eta} d\omega$$

$$= \frac{V_{21} \Delta_{11} + \Delta_{22} - \eta_2}{2} \tanh \left( \frac{\sqrt{(E_{2q \uparrow} - V_{BCS} \gamma)^2 + (\Delta_{11} + \Delta_{22} - \eta_2)^2}}{2kT} \right)$$

$$\text{(7)}$$

Solving for three band model
\[ \Delta_{11} = \left( \frac{V_{12}}{V_{22}} \Delta_{22} + \frac{V_{13}}{V_{33}} \Delta_{33} - \eta_{11} \right) \tanh \left[ \frac{1}{2kT} \left( \Delta_{11} + \frac{V_{12}}{V_{22}} \Delta_{22} + \frac{V_{13}}{V_{33}} \Delta_{33} - \eta_{11} \right) \right] \]

\[ \Delta_{12} = \left( \frac{V_{21}}{V_{11}} \Delta_{11} + \Delta_{22} + \frac{V_{23}}{V_{33}} \Delta_{33} - \eta_{22} \right) \tanh \left[ \frac{1}{2kT} \left( E_{2\gamma}^{+} - V_{BCS}\gamma \right)^{2} + \left( \frac{V_{21}}{V_{11}} \Delta_{11} + \Delta_{22} + \frac{V_{23}}{V_{33}} \Delta_{33} - \eta_{22} \right) \right] \]

\[ \Delta_{13} = \left( \frac{V_{31}}{V_{11}} \Delta_{11} + \Delta_{22} + \Delta_{33} - \eta_{11} \right) \tanh \left[ \frac{1}{2kT} \left( E_{3\gamma}^{+} - V_{BCS}\gamma \right)^{2} + \left( \frac{V_{31}}{V_{11}} \Delta_{11} + \Delta_{22} + \Delta_{33} - \eta_{11} \right) \right] \]

The third correlation function is:

\[ \langle a_{m\uparrow}^{\dagger} a_{n\downarrow}^{\dagger} \rangle = \frac{-1}{i} \int_{-\infty}^{\infty} G_{10}(\omega + iE) - G_{10}(\omega - iE) \frac{e^{i\omega\eta}}{\omega} \, d\omega \]

Now considering the two Green's functions for localized electrons:

\[ G_{i\uparrow}^{\dagger} = \left\langle \langle h_{i\uparrow} h_{i\uparrow} \rangle \right\rangle \] (11a)

\[ G_{i\downarrow}^{\dagger} = \left\langle \langle h_{i\downarrow}^{\dagger} h_{i\downarrow} \rangle \right\rangle \] (11b)

The two equations of motion obtained are:

\[ (\omega - E_{i\uparrow}) G_{1} - \Delta_{M} G_{2} = \frac{1}{2\pi} \]

\[ (\omega + E_{i\downarrow}) G_{2} - \Delta_{M} G_{1} = 0 \]

Taking \( \Delta_{M} = \sum_{mp} \alpha \Delta_{mn} V \) and \( G_{i} = G_{i\uparrow}^{\dagger} \) and \( G_{i} = G_{i\downarrow} \).

The antiferromagnetic order parameter is defined as:

\[ \eta_{m} = \alpha \sum_{p} \left\langle b_{p\uparrow}^{\dagger} b_{p\downarrow} \right\rangle \]

Correlation function is written as:

\[ \left\langle b_{i\uparrow}^{\dagger} b_{j\downarrow} \right\rangle = i \int_{-\infty}^{\infty} \frac{G_{z}(\omega + iE) - G_{z}(\omega - iE)}{e^{i\omega\eta} - 1} \, d\omega \]

Antiferromagnetic order parameter for different number of band models is written as:
\[ \eta_{ir} = \frac{\alpha \sum_r \left( \frac{\alpha \Delta_{AM}}{V_{MM}} \right)}{2 \sqrt{E^2 + \left( \frac{\alpha \Delta_{AM}}{V_{MM}} \right)^2}} \tanh \left( \frac{E^2 + \left( \frac{\alpha \Delta_{AM}}{V_{MM}} \right)^2}{2kT} \right) \]  

(14)

For one band model:

\[ \eta_{11} = N_o \alpha \int_0^{\hbar \omega} \frac{\alpha \Delta_{11}}{V_{11}} \tanh \left( \frac{E^2 + \left( \frac{\alpha \Delta_{11}}{V_{11}} \right)^2}{2kT} \right) \]  

(15)

For two band model:

\[ \eta_{22} = N_o \alpha \int_0^{\hbar \omega} \frac{\alpha \Delta_{11} + \Delta_{22}}{V_{11} + V_{22}} \tanh \left( \frac{E^2 + \alpha^2 \left( \frac{\Delta_{11}}{V_{11}} + \frac{\Delta_{22}}{V_{22}} \right)^2}{2kT} \right) \]  

(16)

For three band model:

\[ \eta_{33} = N_o \alpha \int_0^{\hbar \omega} \frac{\alpha \left( \frac{\Delta_{11}}{V_{11}} + \frac{\Delta_{22}}{V_{22}} + \frac{\Delta_{33}}{V_{33}} \right)}{2 \sqrt{E^2 + \alpha^2 \left( \frac{\Delta_{11}}{V_{11}} + \frac{\Delta_{22}}{V_{22}} + \frac{\Delta_{33}}{V_{33}} \right)^2}} \tanh \left( \frac{E^2 + \alpha^2 \left( \frac{\Delta_{11}}{V_{11}} + \frac{\Delta_{22}}{V_{22}} + \frac{\Delta_{33}}{V_{33}} \right)^2}{2kT} \right) \]  

(17)

3. Results and Discussion

In this study, \( T_C, \eta \) and \( T_M \) for multiband iron pnictides is investigated. The variation of \( T_C \) with \( \eta \) and variation of \( T_M \) with \( \eta \) are studied to obtain the region where both orders, i.e., superconducting and AFM coexist. The region under the two graphs is merged that shows the coexistence of superconductivity and AFM in the system. The problem is solved keeping in mind the multiband nature of pnictides and expressions are obtained for one band, two band and three band models and solved as a function of the number of bands.

Using Equation (5), the variation of \( T_C \) vs \( \eta_{11} \) for one band model is plotted. \textbf{Figure 1} indicates that till about 9 K, as \( \eta_{11} \) increases, \( T_C \) also increases. After 9 K, \( \eta_{11} \) decreases with increasing \( T_C \). At low \( T_C \), \( \eta \) increases, but beyond a critical \( T_C \) of 9 K in the one band model, as \( T_C \) increases, in order to stabilise superconductivity, \( \eta \) decreases.

Using Equation (14), the variation of \( T_M \) vs \( \eta_{11} \) for one band model is plotted. From this graph, it is observed that \( \eta_{11} \) increases with \( T_M \).

Using \textbf{Figure 1} and \textbf{Figure 2}, \( T_C \) and \( T_M \) vs. \( \eta_{11} \) are plotted. The region under the intersection of the two merged graphs demonstrates that superconductivity and AFM coexist in iron pnictides. The area under the curve is found to be 9.44 square units (\textbf{Figure 3}).
Figure 1. $T_c(K)$ vs $\eta_{11}(\text{meV})$ for 1 band model.

Figure 2. $T_m(K)$ vs $\eta_{11}(\text{meV})$ for 1 band model.

Figure 3. $T_c(K)$ and $T_m(K)$ vs $\eta_{11}(\text{meV})$ for 1 band model.
Using Equation (6) and (7), the variation of $T_C$ vs $\eta_{22}$ for two band model is plotted. Figure 4 indicates that till about 35 K, as $\eta_{22}$ increases, $T_C$ also increases. After 35 K, $\eta_{22}$ decreases with increasing $T_C$. At low $T_C$, $\eta$ increases, but beyond a critical $T_C$ of 35 K in the two band model, as $T_C$ increases, in order to stabilise superconductivity, $\eta$ decreases.

Using Equation (15), the variation of $T_M$ vs $\eta_{22}$ for two band model is plotted. From this graph, it is observed that $\eta_{22}$ increases with $T_M$.

Using Figure 4 and Figure 5, $T_C$ and $T_M$ vs $\eta_{22}$ are plotted. The region under the intersection of the two merged graphs demonstrates that superconductivity and AFM coexist in iron pnictides. The area under the curve is found to be 36 square units (Figure 6).

Using Equation (8), (9) and (10), the variation of $T_C$ vs $\eta_{33}$ for 3 band model is plotted. Figure 7 indicates that till about 25 K, as $\eta_{33}$ increases, $T_C$ also increases. After 25 K, $\eta_{33}$ decreases with increasing $T_C$. At low $T_C$, $\eta$ increases, but beyond a critical $T_C$ of 25 K in this model, as $T_C$ increases, in order to stabilise superconductivity, $\eta$ decreases.

Using Equation (16), the variation of $T_M$ vs $\eta_{33}$ for three band model is plotted. From this graph, it is observed that $\eta_{33}$ increases with $T_M$.

Using Figure 7 and Figure 8, $T_C$ and $T_M$ vs $\eta_{33}$ are plotted. The region under the intersection of the two merged graphs demonstrates that superconductivity and AFM coexist in iron pnictides. The area under the curve is found to be 70.68 square units.

The present theoretical study, to an extent has been able to explain the coexistence of superconductivity and magnetism in multiband SmOFeAs superconductor. The compound SmOFeAs upon doping is seen to show both superconductivity and magnetic order [42]. Figure 3, Figure 6 and Figure 9 show the coexistence curves for one, two and three band models respectively.
Figure 5. $T_m$ (K) vs $\eta_{22}$ (meV) for 2 band model.

Figure 6. $T_c$ and $T_m$ (K) vs $\eta_{22}$ (meV) for 2 band model.

Figure 7. $T_c$ vs $\eta_{33}$ for 3 band model.
A common notion that suggests superconductivity and magnetism to be hostile to each other, thus if this was the universal rule, then with \( T_c \) increasing, \( \eta \) should have decreased. In Figure 1, it is seen that till about a critical \( T_c \) of 9 K, both superconductivity and magnetism are seen to support each other, that is with increasing \( T_c \), \( \eta \) also increases for this low value of \( T_c \). The explanation for this kind of unusual trend can be reasoned out from the findings of L. Boeri et al. [43] that talks about electron-phonon coupling. A possible reason could be static magnetism [44] that is independent of doping and is seen to increase the electron phonon coupling constant \( \lambda \), which in turn increases \( T_c \). Also with a strong electron electron interaction in this region, a strong electron electron interaction is seen in the Cooper pair that signifies both the orders to support each other and
in no case superconductivity shows any signs of suppression. Beyond a certain doping, wherein doping can disturb static magnetism which makes $\lambda$ start decreasing. This again makes $T_C$ to decrease with increasing value of $\eta$. Thus a weak electron-phonon coupling exists in this region, showing a weak electron-electron interaction in the Cooper pair that shows both the orders to be hostile to each other, signifying that superconductivity is suppressed.

Beyond the 9 K $T_C$ region in Figure 3, at high values of $T_C$, $\eta$ decreases which shows the usual trend. Similar kind of behaviour is seen in Figure 4 and Figure 7 for two and three band models respectively. The critical $T_C$ for two band model is about 35 K and for the three band model is around 25 K.

Another probable reason for this kind of behaviour of $T_C$ can be seen from the experimental findings of R. M. Fernandes et al. [45] that show how disorder affects the $T_C$ of the s$^+$– superconducting state in iron pnictides. In the under-doped region, superconductivity emerges from a pre-existing magnetic state and disorder gives rise to two competing effects, firstly breaking of the Cooper pairs, that reduces $T_C$ and secondly suppression of the itinerant magnetic order that increases $T_C$. Their findings show that for a wide range of parameters in the coexistence state, $T_C$ can increase with disorder.

In Figure 2, Figure 5 and Figure 8, $T_M$ vs $\eta$ for one, two and three band models respectively is shown. It is observed that $\eta$ increases with $T_M$. In the curves at a certain $T_M$ about 9 K for one band model, 11 K for two band model and 25 K for three band model, an abrupt slight increase in the value of $\eta$ with $T_M$ is seen. This unusual trend is attributed to the sharp peak that is observed in the specific heat curve due to AFM ordering of Sm$^{3+}$ magnetic ions in the system which is otherwise not seen in the lanthanum compound that has non-magnetic La$^{3+}$ ions [46].

Comparing the data of one, two and three band models, it is seen that with increasing number of bands, the coexistence region increases as is evident from the combined graph of $T_C$ vs $\eta$ and $T_M$ vs $\eta$, thereby showing that the material can withhold a larger value of magnetic field upon increasing the number of bands.

4. Conclusions

Iron pnictides are a special class of superconductors. In the present research work, the doped samarium iron pnictide compound SmOFeAs is theoretically studied. Also earlier studies on the effect of multiband structure on critical temperature and electronic specific heat in SmOFeAs iron pnictide superconductor has been studied by Shamin Masih et al. [47]. In this research work, theoretical calculations are made until the three band model as Ummarino has suggested that a simple three band model in strong-coupling regime can reproduce in a quantitative way the experimental $T_C$. From the findings of R. M. Fernandes et al. on unconventional pairing in the iron arsenide superconductors, the results show theoretically that AFM and superconductivity can coexist in these mate-
rials only if Cooper pairs form an unconventional, sign-changing state. Also their study finds that AFM and conventional phonon-mediated superconductivity cannot coexist. Therefore unconventional s+− pairing is located near the borderline between phase coexistence and mutual exclusion. Their findings strongly suggest that superconductivity is unconventional in iron pnictides. This study further points out that correlation between superconductivity and magnetism doesn’t change with increasing number of bands.

To conclude this work, one can say that the study has given insight into how these multiband structures behave and how the possibility for coexistence increases making the material more robust in nature. Attempt has been made to give explanations for both the regular and anomalous behaviors of the parameters under study.

Conflicts of Interest

The authors declare no conflicts of interest.

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