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The Coexistence of Super Conductivity and Spin Density Wave (SDW) in $SmO_{1-x}F_xFeAs$

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Abstract

The coexistence of superconductivity and spin density wave in $SmO_{1-x}F_xFeAs$ is theoretically studied using the model Hamiltonian which contains BCS type superconductivity and spin density wave terms. Employing green function formalism, the expression for the spin density wave order parameter (M) and expression for spin density wave transition temperature T_{SDW} is obtained. The interplay between the superconductivity and spin density wave is examined in these parameters and the coexistence of the two states is established in the order parameter range of $0.1 \leq M \leq 0.137$ meV which is seen to be in broad experimental agreement.

Keywords

Coexistence, Superconducting Order Parameter, Spin Density Wave Order Parameter and Green Function

1. Introduction

The discovery superconductivity with a transition temperature of 26 K in $LaO_{1-x}F_xFeAs$ system [1] has generated tremendous interest in the scientific community. Shortly after this discovery, several groups reported an increase of T_c values by replacing La with smaller-size rare-earth ions (T_c = 41 K in $CeO_{1-x}F_xFeAs$ [2], T_c = 52 K in $NdO_{1-x}F_xFeAs$ [3], T_c = 52 K in $PrO_{1-x}F_xFeAs$ [4] [5] and the substitution of La with Sm, T_c was found to be 55 K in $SmO_{1-x}F_xFeAs$ [6] [7].

Besides a relative high T_c, the system displays many interesting properties. First, they promise interesting physics that stem from the coexistence of superconductivity and magnetism. Second, they provide a much wider variety of compounds for research and, with their multi-band electronic structure; they offer the hope of finally discovering the mechanism of high temperature superconductivity and finding the way to increase T_c [8].

The parent compounds of these materials are itinerant spin density wave magnetic order or anti ferromagnetic

order [9] [10]. Superconductivity emerges when doping a magnetic mother compound with electron or holes and thereby suppressing the magnetic order [9] [11]. The proximity of the superconductivity state to the spin density wave phase in the phase diagram implies that the interplay between the magnetism and superconductivity might play an important role in understanding the pairing mechanism and other physical properties of the iron-based superconductors. It is generally believed that the magnetic couplings between the itinerant electrons and/or between the itinerant electron and local spin are essential to both spin density wave instability and superconductivity.

The Muon spin rotation study on the newly discovered iron pnictide superconductor found that magnetism and superconductivity coexist in the long rang doping in $SmO_{1-x}F_xFeAs$ $(0.1 \leq x \leq 0.13)$ [12].

In the present work we study theoretical coexistence of superconductivity and spin density wave in $SmO_{1-x}F_xFeAs$. The model of the Hamiltonian used in describing the system incorporate two competing physical processes involving the electron hole like pairing and electron-electron pairing. The results of our work clearly show that over certain order parameter range superconductivity and spin density wave are established.

2. Formulation of the Problem

The model of the Hamiltonian for coexistence spin density wave and superconductivity in our compound can be describe as

$$H = H_1 + H_2 \tag{1}$$

where $H_1 = \sum_{p\sigma} \epsilon_p \hat{a}_{p\sigma}^+ \hat{a}_{p\sigma} + \Delta_{sc} \sum_p \hat{a}_{p\uparrow}^+ \hat{a}_{-p\downarrow}^+ + \hat{a}_{-p\downarrow} \hat{a}_{p\uparrow}$, the first term of H_1 represent single particle energies of

the conduction and the second term BCS type electron-electron pairing; $H_2 = M \sum_p \left(\hat{a}_{p+q\uparrow}^+ \hat{a}_{p\downarrow} + \hat{a}_{p\downarrow}^+ \hat{a}_{p+q\uparrow} \right)$ is

spin density wave Hamiltonian term; $\left(\hat{a}_{p\sigma}^+ \hat{a}_{p\sigma} \right)$ are the creation (annihilation) operators of an electron having

the wave number k and spin σ.

$\Delta_{sc} = -V \sum_k \left\langle \hat{a}_{-k\downarrow} \hat{a}_{k\uparrow} \right\rangle = -V \sum_k \left\langle \hat{a}_{k\uparrow}^+ \hat{a}_{-k\downarrow}^+ \right\rangle$ is superconducting order parameter; $M = -U \sum_k \left\langle \hat{a}_{k\uparrow}^+ \hat{a}_{k-q\downarrow} \right\rangle$ is the

spin density wave order parameters.

The double-time temperature dependent retarded Green function is given by (Zubarev) [13]

$$G_r(t-t') = \left\langle\left\langle \hat{A}(t), \hat{B}(t) \right\rangle\right\rangle_r = -i\theta(t-t') \left\langle \left[\hat{A}(t), \hat{B}(t') \right] \right\rangle \tag{2}$$

where $\left\langle\left\langle \cdots \right\rangle\right\rangle$ is abbreviated notation for the corresponding the Green's function and $\left\langle \cdots \right\rangle$ indicates the average over a grand canonical ensemble for the operators. $\theta(t-t')$ is Heaviside step function, $\hat{A}(t), \hat{B}(t)$ are operators in Heisenberg picture.

$\left[\hat{A}(t), \hat{B}(t) \right]$ is a commutator or anticommutator.

To find the equation of motion for the Green's function, differentiating Equation (2) with respect to time and, we get

$$\frac{i\mathrm{d}G_r(t-t')}{\mathrm{d}t} = \frac{\mathrm{d}}{\mathrm{d}t}\theta(t-t') \left\langle \left[\hat{A}(t), \hat{B}(t') \right] \right\rangle + i\frac{\mathrm{d}}{\mathrm{d}t} \left\langle\left\langle \hat{A}(t), \hat{B}(t) \right\rangle\right\rangle \tag{3}$$

The relation between Heaviside step function $\theta(t)$ and Dirac delta function δ is given by

$$\frac{\mathrm{d}}{\mathrm{d}t}\theta(t-t') = \delta(t-t') \tag{4}$$

The equation of motion expresses as,

$$\frac{i\mathrm{d}\hat{A}(t)}{\mathrm{d}t} = \left[\hat{A}(t), \hat{H} \right] \tag{5}$$

Based on the relation between Heaviside step function $\theta(t)$ and Dirac delta function δ, Equation (3) can

be written as

$$\frac{i\mathrm{d}G_r(t-t')}{\mathrm{d}t} = \left\langle \left[\hat{A}(t), \hat{B}(t') \right] \right\rangle + \left\langle \left\langle \left[\hat{A}(t), H \right], \hat{B}(t) \right\rangle \right\rangle \tag{6}$$

The Fourier transformation of $G_r(t-t')$

$$G_r(t-t') = \int_{-\infty}^{\infty} G_r(\omega) \mathrm{e}^{-\omega(t-t')} \tag{7}$$

Considering delta function, the derivative of Equation (7) become

$$\frac{\mathrm{d}G_r(t-t')}{\mathrm{d}t} = -i\omega X \cdot G_r(\omega) \tag{8}$$

Comparing Equation (6) and (8), we get

$$\omega = \left\langle \left\langle \hat{A}(t), \hat{B}(t) \right\rangle \right\rangle = \left\langle \left[\hat{A}(t), \hat{B}(t') \right] \right\rangle_\omega + \left\langle \left\langle \left[\hat{A}(t), H \right], \hat{B}(t) \right\rangle \right\rangle_\omega \tag{9}$$

2.1. Dependence of SDW (M) on the Superconductivity Critical Temperature (T$_c$)

The equation of motion for the correlation $\left\langle \left\langle \hat{a}_{k\uparrow}^+, \hat{a}_{-k\downarrow}^+ \right\rangle \right\rangle$ can be written as;

$$\omega \left\langle \left\langle \hat{a}_{k\uparrow}^+, \hat{a}_{-k\downarrow}^+ \right\rangle \right\rangle = \left\langle \left\langle \left[\hat{a}_{k\uparrow}^+, H \right], \hat{a}_{-k\downarrow}^+ \right\rangle \right\rangle \tag{10}$$

Solving the commentator in Equation (10), we get

$$\left\langle \left\langle \hat{a}_{k\uparrow}^+, \hat{a}_{-k\downarrow}^+ \right\rangle \right\rangle = \frac{-1/2(\Delta_{sc} + M)}{\omega^2 + \epsilon_k^2 + (\Delta_{sc} + M)^2} + \frac{-1/2(\Delta_{sc} - M)}{\omega^2 - \epsilon_k^2 - (\Delta_{sc} - M)^2} \tag{11}$$

Using the expression $\omega \to i\omega$ and Matsubara's frequency, we have

$$\left\langle \left\langle \hat{a}_{k\uparrow}^+, \hat{a}_{-k\downarrow}^+ \right\rangle \right\rangle = \frac{1}{2} \sum_{j=1,2} \frac{\beta^2 \Delta_j(k)}{(2n+1)^2 \pi^2 + \beta^2 \left(\epsilon^2 + \Delta_j^2(k) \right)} \tag{12}$$

Thus, the superconductivity order parameter Δ_{sc} can be expressed as follows

$$\Delta_{sc} = \frac{V}{2} \sum_{k,nj=1,2} \frac{\beta^2 \Delta_j(k)}{(2n+1)^2 \pi^2 + \beta^2 \left(\epsilon^2 + \Delta_j^2(k) \right)} \tag{13}$$

Let us employ the following equality relation below to solve the superconductivity order parameter

$$\sum_{-\infty}^{\infty} \frac{1}{(2n+1)^2 \pi^2 + \gamma^2} = \frac{\tanh \gamma/2}{2\gamma} \quad \text{where} \quad \gamma = \beta \left(\epsilon^2 + \Delta_j^2(k) \right)^{\frac{1}{2}} \tag{14}$$

Using the above equality relation, the superconducting order parameter can be expressed as

$$\Delta_{sc} = \frac{V}{4} \sum_{k,j=1,2} \frac{\Delta_j(k) \tanh \frac{\beta}{2} \left(\epsilon^2 + \Delta_j^2(k) \right)^{\frac{1}{2}}}{\left(\epsilon^2 + \Delta_j^2(k) \right)^{\frac{1}{2}}} \tag{15}$$

Converting the summation over k values into an integral by introducing the density of state $N(o)$, we can write superconducting order parameter as

$$\Delta_{sc} = \lambda \int_0^{\hbar\omega_b} (\Delta_{sc} - M) \frac{\tanh \frac{\beta}{2} \left(\epsilon_k^2 + (\Delta_{sc} - M)^2 \right)^{\frac{1}{2}}}{\left(\epsilon_k^2 + (\Delta_{sc} - M)^2 \right)^{\frac{1}{2}}} \mathrm{d}\epsilon_k \tag{16}$$

After rearranging Equation (16), we get

$$\frac{1}{\lambda} = \int_0^{\hbar\omega_b} \left(1 - \frac{M}{\Delta_{sc}}\right) \frac{\tanh\frac{\beta}{2}\left(\epsilon_k^2 + (\Delta_{sc} - M)^2\right)^{\frac{1}{2}}}{\left(\epsilon_k^2 + (\Delta_{sc} - M)^2\right)^{\frac{1}{2}}} \, d\epsilon_k \tag{17}$$

We consider the case, when $T \to 0, \beta \to \infty$, then the SDW can be expressed as

$$M = 1.75 k_\beta T_c - 2\hbar\omega_b \exp\left(-\frac{1}{\lambda\left(1 - \dfrac{M}{1.75 k_\beta T_c}\right)}\right) \tag{18}$$

2.2. Dependence of SDW (M) on the SDW Transition Temperature (T$_{SDW}$)

The equation of motion for the correlation $\left\langle\left\langle \hat{a}_{k\uparrow}^+, \hat{a}_{k-q\downarrow} \right\rangle\right\rangle$ to express the order parameter of SDW can be described as:

$$\omega\left\langle\left\langle \hat{a}_{k\uparrow}^+, \hat{a}_{k-q\downarrow} \right\rangle\right\rangle = \left\langle\left\langle \left[\hat{a}_{k\uparrow}^+, H\right], \hat{a}_{k-q\downarrow} \right\rangle\right\rangle \tag{19}$$

Evaluating the commutation in Equation (19), we obtain

$$\left\langle\left\langle \hat{a}_{k\uparrow}^+, \hat{a}_{k-q\downarrow} \right\rangle\right\rangle = \frac{-M\left[\omega^2 - f_k^2 - M^2 + \Delta_{sc}^2\right]}{\left[\omega^2 - f_k^2 - (\Delta_{sc} + M)^2\right]\left[\omega^2 - f_k^2 - (\Delta_{sc} - M)^2\right]} \tag{20}$$

Using the expression $\omega \to i\omega$ and Matsubara's frequency, we get

$$\left\langle\left\langle \hat{a}_{k\uparrow}^+, \hat{a}_{k-q\downarrow} \right\rangle\right\rangle = \frac{1}{2}\sum_{j=1,2} \frac{(-1)^j \beta^2 \Delta_{sc}(k)}{(2n+1)^2 \pi^2 + \beta^2\left(\epsilon^2 + \Delta_j^2(k)\right)} \tag{21}$$

Thus, the SDW order parameter is given by

$$M = -\frac{U}{2}\sum_{j=1,2} \frac{\beta\Delta_{sc}(k)}{(2n+1)^2 \pi^2 + \beta^2\left(\epsilon^2 + \Delta_j^2(k)\right)}, \tag{22}$$

Using the equality relation in Equation (14), the SDW order parameter can be expressed as

$$M = -\frac{U}{4}\sum_{j=1,2} \frac{\Delta_j(k)\tanh\frac{\beta}{2}\left(\epsilon^2 + \Delta_j^2(k)\right)^{\frac{1}{2}}}{(2n+1)^2 \pi^2 + \beta^2\left(\epsilon^2 + \Delta_j^2(k)\right)} \tag{23}$$

Changing of the summation into an integral by introducing the density of state $N(o)$, we obtained the expression for SDW order parameter as

$$M = \frac{-N(O)_j U}{2} \int_0^{\hbar\omega_b} \frac{\Delta_j(k)\tanh\frac{\beta}{2}\left(\epsilon^2 + \Delta_j^2(k)\right)^{\frac{1}{2}}}{\left(\epsilon^2 + \Delta_j^2(k)\right)^{\frac{1}{2}}} \, d\epsilon_k \tag{24}$$

After simplifying the above equation, we obtained

$$M = -\lambda_j \Delta_j \left(\left(\ln 1.14\frac{\hbar\omega_b}{k_\beta T_{SDW}}\right) - \Delta_j^2\left(\frac{1}{\pi k_\beta T_{SDW}}\right)^2 1.052\right) \tag{25}$$
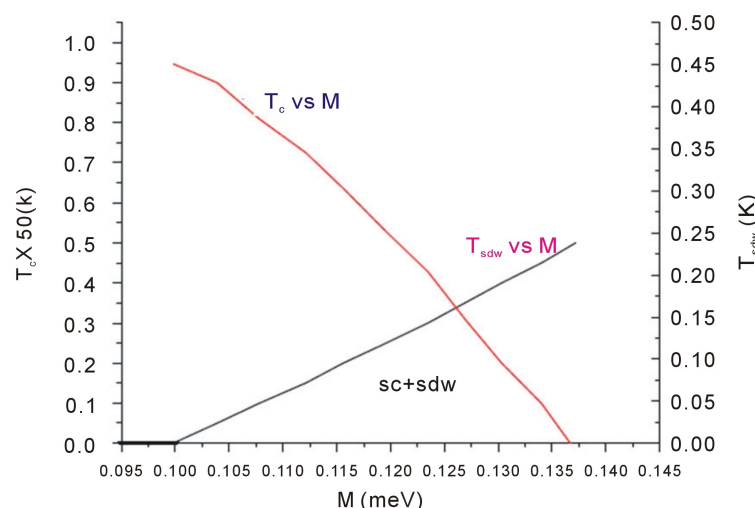
Figure 1. The T_c and T_{SDW} vs. magnetic order parameter.

where $\lambda_j = N(O)_j U$.

For very small value of Δ_j the second term of the RHS of Equation (25) goes to zero. Thus, for $\Delta_j = 0$ SDW transition temperature can be written as

$$T_{sdw} = 1.14 \frac{\hbar\omega_b}{k_\beta} \exp\left(\frac{M}{\lambda_j \Delta_j}\right) \tag{26}$$

3. Result and Discussion

Using the model of the Hamiltonian and green function formalism we obtained two important results expressed by Equations (18) and (26). We examined the effect of magnetic order parameter (M) on superconducting transition temperature (T_c) and magnetic order parameter (M) on spin density wave transition temperature (T_{SDW}) in $SmO_{1-x}F_xFeAs$ by using the results. Based on Equation (18), we plotted the phase diagram of T_c versus M which shows that as the magnetic order parameter (M) increases the superconducting transition temperature (T_c) decreases. The phase diagram of magnetic ordering temperature (T_{SDW}) versus magnetic ordering (M) is also plotted based on the Equation (26). As we observed from this graph the magnetic transition temperature increases as the magnetic order parameter increases. Finally when phase diagram of T_c versus M and the phase diagram of T_{SDW} versus M are merged an intersecting region in some range of order parameter is found as indicated in **Figure 1**.

4. Conclusion

Superconductivity and magnetism are antagonistic to each other. However, Muon spin rotation experiment has shown that these two stats coexist in $SmO_{1-x}F_xFeAs$. We are motivated by this experiment and use a model of Hamiltonian and employ green function formalism. We have got mathematical expressions for the order parameters. The intersection region we found under the superconducting critical temperature and SDW transition temperature vs. magnetic order parameter by using these results confirms that these two exclusive phenomena can coexist together in some range of magnetic order as demonstrated in **Figure 1**. Our theoretical predictions are in broad agreement with experimental finding.

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