Coexistence of spin density wave and superconductivity in $BaFe_{2-x}Co_xAs_2$

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Abstract

The relationship between the spin density wave (SDW) and superconductivity is a central topic in the research on the FeAs-based high TC superconductors. In this research work, the theoretical investigation of the coexistence of spin density wave and superconductivity in $BaFe_{2-x}Co_xAs_2$ has been made. By developing a model Hamiltonian for the system and using quantum field theory Green function formalism, we have found mathematical expressions for superconducting transition temperature (Tc), spin density wave transition temperature (Tsdw), superconductiviy order parameter (Δsc) and spin density wave order parameter (Δsdw). The phase diagrams of superconducting transition temperature versus superconductiviy order parameter and spin density wave transition temperature versus spin density wave order parameter have been plotted. By combining the two phase diagrams, we have obtained a phase diagram which shows the possible coexistence of spin density wave and superconductivity in $BaFe_{2-x}Co_xAs_2$.

Keywords: Spin density wave, Superconductivity, Spin density wave order parameter, Superconductivity order parameter, Coexistence of spin density wave, Superconductivity.

Resumen

La relación entre la onda de densidad de espín (SDW) y la superconductividad es un tema central en la investigación sobre los superconductores de alta TC basados en FeAs. En este trabajo se ha realizado la investigación teórica de la coexistencia de onda de densidad de espín y la superconductividad en BaFe2-xCoxAs2. Mediante el desarrollo de un modelo de Hamilton para el sistema y el uso de la teoría del campo cuántico en función formalismo de Green, hemos encontrado expresiones matemáticas para la temperatura de transición superconductora (Tc), para la temperatura de transición de la densidad de onda del espín (Tsdw), para el parámetro de orden de la superconductividad (Δsc) y el parámetro de densidad de onda del espín (Δsdw). Se elaboraron los diagramas de fase de la temperatura de transición superconductora contra el parámetro de orden de la superconductividad y la temperatura de transición de la densidad de espín contra el parámetro de orden de la densidad de onda del espín. Mediante la combinación de los dos diagramas de fase, hemos obtenido otro diagrama de fase que muestra la posible coexistencia de onda de densidad del espín y la superconductividad del BaFe2-xCoxAs2.

Palabras clave: Densidad de onda del espín, Superconductividad, Parámetros de orden de la densidad de onda de espín, Parámetros para la superconductividad, Coexistencia de densidad de onda del espín y la superconductividad.

I. INTRODUCTION

Superconductivity is a phenomenon which is manifested by certain conductors that demonstrate no resistance to the flow of currents. Superconductors also exhibit strong diamagnetism which expel magnetic fields from their interior. The first widely accepted theoretical formulation of conventional superconductivity was forwarded in 1957 by John Bardeen, Leon Cooper and John Schrieffer which is nowadays known as the BCS theory. The BCS theory explains superconductivity at temperatures close to absolute zero for some elements and alloys. However, at higher temperatures and with different superconducting systems, the BCS theory has subsequently became inadequate to explain how superconductivity occurs [1]. The decade of 1980 were years of unrivaled discovery in the field of superconductivity. In 1964, Bill Little had suggested the possibility of organic or Carbon-based superconductors [2].

The first of these superconductors was successfully synthesized in 1980 by Klaus Bechgard and three French team members [2]. In 1986, a discovery was made in the field of high temperature superconductors. Alex Muller and George Bednorz discovered a brittle ceramic compound that superconducts at a temperature of about 36K [3].

In 1997 researchers found that, at a temperature very near to the absolute zero, alloys of gold and indium were both superconductors and a natural magnet.

The Spin Density Wave (SDW) state is a kind of antiferromagnetic state with the electronic spin density forming a static wave. It occurs at low temperature in anisotropic low dimensional materials.

Spin density wave (SDW) couples to the spin. It refers to the periodic modulation of spin density with a period (T) determined by the Fermi wave number [4].

The density varies perpendicularly as a function of position with no net magnetization in the entire volume. In the normal state, the density $\rho_\uparrow(r)$ of electron spins polarized upward with respect to any quantization axis is completely deleted by $\rho_\downarrow(r)$ of downward polarized spins. Therefore, their difference is finite and modulate in space as a function of the position vector in the spin density wave state [5].

BaFe$_{2-x}$Co$_x$As$_2$ superconductivity was observed up to a maximum critical temperature of, T_C=25K [6, 7]. This compound is known as Ba-122.

There are two major families of FeAs superconductors that have been investigated as REOFeAs systems, broadly termed as 1111 compounds [8], where RE is rare-earth and the two layered AFe$_2$As$_2$ systems, termed as the 122 compounds [9], where A stands for an alkaline earth elements such as Ca, Sr, Ba or the divalent rare earth metals.

Like in oxypnictides, the crystal structure is layered and formed by edge sharing FeAs4/4 tetrahedrons with covalent bonding, interlaced by the layers of Ba^{2+} sheets perpendicular to 001 instead of (La-O) layers for LaOFeAs.

Like oxypnictides, the interlayer bonding is ionic. The metal-metal bonding within the layers plays an important role in the properties of ThCr$_2$Si$_2$ type structure.

The iron atoms are in the Fe^{2+} state (3d^6) the d-shell is more than half filled and Fe-Fe antibonding states should be at least partially occupied. The distance between the nearest Fe atoms within FeAs layers is also significantly smaller in AFe$_2$As$_2$ as compared to the LaOFeAs system.

The superconductivity of AFeAs based superconductors are not associated with oxygen layers but it does not break the monopoly of cuprates which means it does not contain oxygen. The differences between the two systems regarding structural and magnetic transition are in oxypnictide both the structural and magnetic transition occur at different temperatures.

The magnetic transition occurs between 10K and 20K lower than the structural transition while in AFe$_2$As$_2$ compounds, it is found coupled and for same transition temperature [10].

II. THEORETICAL MODEL SYSTEM HAMILTONIAN

We consider the following model hamiltonian:

$$H = \sum_{k'\sigma} \varepsilon_{k'} c^+_{k'\sigma} c_{k'\sigma} + \Delta_{sc} \sum_{k'} \{ c^+_{k'\uparrow} c^+_{-k'\downarrow} + c_{-k'\downarrow} c_{k'\uparrow} \}$$

$$+ \Delta_{sdw} \sum_{k'q} \{ c^+_{(k'+q)\uparrow} c_{k'\downarrow} + c^+_{k'\downarrow} c_{(k'+q)\uparrow} \}, \tag{1}$$

where the first term is the hamiltonian of the free charge carriers (H_0), the second and the third terms denote the superconducting state (H_{sc}) and the spin density wave state (H_{sdw}) respectively.

The superconducting state order parameter (Δ_{sc}) and spin density wave order parameter (Δ_{sdw}) are expressed as:

$$\Delta_{sc} = V \sum_k < c^+_{-k\downarrow} c_{k\uparrow} > .$$

$$\Delta_{sdw} = U \sum_k < c^+_{k\uparrow} c_{(k-q)\downarrow} > .$$

Where $c^+_{k,\sigma} (c_{k,\sigma})$ are creation (annihilation) fermion operators.

Now, let us define:

$$G^{\uparrow\uparrow}_{k'k} = << c_{k\uparrow} c^+_{k\uparrow} >> .$$

Thus, the equation of motion becomes:

$$\omega << c_{k\uparrow} c^+_{k'\uparrow} >> = < [c_{k\uparrow}, c^+_{k'\uparrow}] + << [c_{k\uparrow}, H], c^+_{k'\uparrow} >> . \tag{2}$$

Using the anticommutation relation for creation (annihilation) operators, we get:

i) For the free electron case, we have:

$$[c_{k\uparrow}, H_0] = \varepsilon_k c_{k\uparrow} . \tag{3}$$

ii) For the superconducting part:

$$[c_{k\uparrow}, H_{sc}] = \Delta_{sc} c^+_{-k\downarrow} . \tag{4}$$

iii) Similarly for the *SDW* part, we get:

$$[c_{k\uparrow}, H_{sdw}] = \Delta_{sdw} c^+_{(k-q)\uparrow} . \tag{5}$$

Substituting Equations (3), (4) and (5), into Equation (2), we get:

$$<< c_{k\uparrow}c_{k\uparrow}^{+} >> = \frac{1}{\omega - \varepsilon_k}\{1 + \Delta_{sc} << c_{-k\downarrow}^{+}c_{k\uparrow}^{+} >> \tag{6}$$

$$+\Delta_{sdw} << c_{(k-q)\downarrow}c_{k\uparrow}^{+} >>\}.$$

Similarly, employing the same method as above, we get:

$$<< c_{-k\downarrow}^{+}c_{k\uparrow}^{+} >> = \frac{1}{\omega + \varepsilon_k}\{\Delta_{sc} << c_{k\uparrow}c_{k\uparrow} >> \tag{7}$$

$$-\Delta_{sdw} << c_{(k-q)\downarrow}c_{k\uparrow}^{+} >>.$$

$$<< c_{(k-q)\downarrow}^{+}c_{k\uparrow}^{+} >> = \tag{8}$$

$$-\frac{1}{\omega - \varepsilon_{k-q}}\{-\Delta_{sc} << c_{(k-q)\uparrow}c_{k\uparrow}^{+} >> +\Delta_{sdw} << c_{k\uparrow}c_{k\uparrow}^{+} >>\}.$$

$$<< c_{(k-q)\downarrow}^{+}c_{k\uparrow}^{+} >> = \frac{1}{\omega + \varepsilon_{k-q}}\{\Delta_{sc} << c_{(k-q)\downarrow}c_{k\uparrow}^{+} >> \tag{9}$$

$$+\Delta_{sdw} << c_{-k\uparrow}c_{k\uparrow}^{+} >>\}.$$

Now substituting Equations (6) and (9) into Equation (7), we get:

$$<< c_{-k\downarrow}^{+}c_{k\uparrow}^{+} >> -\{\frac{\Delta_{sc}\Delta_{sdw}\alpha}{\chi}\} << c_{(k-q)\downarrow}c_{k\downarrow}^{+} >>$$
$$= \frac{\Delta_{sc}(\omega + \varepsilon_{k-q})}{\chi}. \tag{10}$$

Where:

$$\alpha = \omega + \varepsilon_{k-q} + \omega - \varepsilon_k.$$

And:

$$\chi = (\omega^2 - \varepsilon_k^2)(\omega + \varepsilon_{k-q}) - \{\Delta_{sc}^2(\omega + \varepsilon_{k-q})$$

$$+\Delta_{sdw}^2(\omega - \varepsilon_k)\}.$$

Similarly, substituting Equations (6) and (9) into Equation (8), we get:

$$\frac{-\Delta_{sc}\Delta_{sdw}\alpha}{\chi} << c_{-k\downarrow}^{+}c_{k\downarrow}^{+} >> + << c_{(k-q)\downarrow}c_{k\uparrow}^{+} >>$$

$$= \frac{\Delta_{sdw}(\omega + \varepsilon_{k-q})}{\chi}. \tag{11}$$

Let M and R be the matrices representation of the system of the linear equation.

$$M = \begin{pmatrix} 1 & \dfrac{-\alpha\,\Delta_{sc}\Delta_{sdw}}{\chi} \\ \dfrac{-\alpha\Delta_{sc}\Delta_{sdw}}{\chi} & 1 \end{pmatrix}. \tag{12}$$

$$R = \begin{pmatrix} \dfrac{\Delta_{sc}(\omega + \varepsilon_{k-q})}{\chi} \\ \dfrac{\Delta_{sdw}(\omega + \varepsilon_{k-q})}{\chi} \end{pmatrix}. \tag{13}$$

The determinant of Equation (13) is given by:

$$\det M = \frac{\chi^2 - (\alpha\Delta_{sc}\Delta_{sdw})^2}{\chi^2}. \tag{14}$$

Substituting, the first column of matrix M by the column of matrix R and denoting the new matrix by M_1 such that:

$$M_1 = \begin{pmatrix} \dfrac{\Delta_{sc}(\omega + \varepsilon_{k-q})}{\chi} & -\dfrac{\alpha\,\Delta_{sc}\Delta_{sdw}}{\chi} \\ \dfrac{\Delta_{sdw}(\omega + \varepsilon_{k-q})}{\chi} & 1 \end{pmatrix}. \tag{15}$$

The determinant of Equation (16) is given by:

$$\det M_1 = \frac{\chi\Delta_{sc}(\omega + \varepsilon_{k-q}) + \alpha\Delta_{sc}\Delta_{sdw}^2(\omega + \varepsilon_{k-q})}{\chi^2}. \tag{16}$$

$$M_2 = \begin{pmatrix} 1 & \dfrac{\Delta_{sc}(\omega + \varepsilon_{k-q})}{\chi} \\ \dfrac{-\alpha\,\Delta_{sc}\Delta_{sdw}}{\chi} & \dfrac{\Delta_{sdw}(\omega + \varepsilon_{k-q})}{\chi} \end{pmatrix}. \tag{17}$$

The determinant of M_2 becomes:

$$\det M_2 = \frac{\chi\Delta_{sdw}(\omega + \varepsilon_{k-q}) + \alpha\Delta_{sc}^2\Delta_{sdw}(\omega + \varepsilon_{k-q})}{\chi^2}. \tag{18}$$

Using Equations (16) and (18), we can determine the value of $<< c_{-k\downarrow}^{+}c_{k\uparrow}^{+} >>$ as follows:

$$<< c_{-k\downarrow}^{+}c_{k\uparrow}^{+} >> = \frac{\det M_1}{\det M}$$

$$= \frac{\chi\Delta_{sc}(\omega + \varepsilon_{k-q}) + \alpha\Delta_{sc}\Delta_{sdw}^2(\omega + \varepsilon_{k-q})}{\chi^2 - (\alpha\Delta_{sc}\Delta_{sdw})^2}.$$

From which get:

$$<< c_{-k\downarrow}^{+} c_{k\uparrow}^{+} >> = \frac{1}{2} \{ \frac{-(\Delta_{sc} + \Delta_{sdw})}{(\omega^2 - \varepsilon_k^2) - (\Delta_{sc} + \Delta_{sdw})^2}$$

$$- \frac{(\Delta_{sc} - \Delta_{sdw})}{(\omega^2 - \varepsilon_k^2) - (\Delta_{sc} - \Delta_{sdw})^2} \}. \tag{19}$$

Using Equations (14) and (18), we can determine the value of $<< c_{(k-q)\downarrow} c_{k\uparrow}^{+} >>$ as follows:

$$<< c_{(k-q)\downarrow} c_{k\uparrow}^{+} >> = \frac{\det M_2}{\det M} =$$

$$\frac{\chi \Delta_{sdw}(\omega + \varepsilon_{k-q}) + \alpha \Delta_{sc}^2 \Delta_{sdw}(\omega + \varepsilon_{k-q})}{\chi^2 - (\alpha \Delta_{sc} \Delta_{sdw})^2}.$$

From which we get:

$$<< c_{(k-q)\downarrow} c_{k\uparrow}^{+} >> = \frac{1}{2} \{ \frac{\Delta_{sc} + \Delta_{sdw}}{(\omega^2 - \varepsilon_k^2) - (\Delta_{sc} + \Delta_{sdw})^2}$$

$$+ \frac{\Delta_{sc} - \Delta_{sdw}}{(\omega^2 - \varepsilon_k^2) - (\Delta_{sc} - \Delta_{sdw})^2} \}. \tag{20}$$

A. The order parameter of superconductivity

The superconducting order parameter (Δ_{sc}) can be obtained using:

$$\Delta_{SC} = \frac{V}{\beta} \sum_k << c_{-k\downarrow}^{+} c_{k\uparrow}^{+} >>, \tag{21}$$

where $\beta = (k_B T)^{-1}$ and k_B is the Boltzmann constant.

Substituting Equation (19) into Equation (21), we get:

$$\Delta_{sc} = \frac{V}{2\beta} \sum_{k,n} \{ \frac{-(\Delta_{sc} + \Delta_{sdw})}{(\omega_n^2 - \varepsilon_k^2) - (\Delta_{sc} + \Delta_{sdw})^2} \tag{22}$$

$$- \frac{(\Delta_{sc} - \Delta_{sdw})}{(\omega_n^2 - \varepsilon_k^2) - (\Delta_{sc} - \Delta_{sdw})^2} \}.$$

Where ω_n is the Matsubara frequency, which is given by:

$$\omega_n = \sum_n \frac{\pi(2n+1)}{\beta}. \tag{23}$$

Substituting Equation (23) into Equation (22), we obtain:

$$\Delta_{sc} = \frac{V}{2\beta} \sum_{n,k} \{ \frac{-(\Delta_{sc} + \Delta_{sdw})}{(\pi(2n+1))^2 - \beta^2(\varepsilon_k^2 + (\Delta_{sc} + \Delta_{sdw})^2)}$$

$$- \frac{(\Delta_{sc} - \Delta_{sdw})}{(\pi(2n+1))^2 - \beta^2(\varepsilon_k^2 + (\Delta_{sc} - \Delta_{sdw})^2)} \}. \tag{24}$$

By changing the summation into integration and by introducing the density of states, $N(0)$, Equation (24) can be expressed as:

$$\Delta_{sc} = \beta V N(0) \sum_n \int_0^{\hbar\omega} \{ \frac{\Delta_{sc} + \Delta_{sdw}}{(\pi(2n+1))^2 + (\beta\varepsilon)^2} +$$

$$\frac{\Delta_{sc} - \Delta_{sdw}}{(\pi(2n+1))^2 + (\beta\varepsilon')^2} \} d\varepsilon. \tag{23}$$

Where:

$$\varepsilon^2 = \varepsilon_k^2 + (\Delta_{sc} + \Delta_{sdw})^2.$$

$$\varepsilon'^2 = \varepsilon_k^2 + (\Delta_{sc} - \Delta_{sdw})^2.$$

Now, let us define:

$$\tan h(\beta\varepsilon/2)/2\beta\varepsilon = \sum_n \frac{1}{(\pi(2n+1))^2 + (\beta\varepsilon)^2}. \tag{26}$$

And:

$$\tan h(\beta\varepsilon'/2)/2\beta\varepsilon' = \sum_n \frac{1}{(\pi(2n+1))^2 + (\beta\varepsilon')^2}. \tag{27}$$

Using Equations (26) and (27) in Equation (25), we get:

$$\Delta_{sc} = \beta V N(0) \int_0^{\hbar\omega_F} \{ (\Delta_{sc} + \Delta_{sdw}) \tan h(\beta\varepsilon/2)/2\beta\varepsilon$$

$$+ (\Delta_{sc} - \Delta_{sdw}) \tan h(\beta\varepsilon'/2)/2\beta\varepsilon' \} d\varepsilon. \tag{28}$$

$$\frac{2}{\lambda} = \int_0^{\hbar\omega_F} \{ (1 + \frac{\Delta_{sdw}}{\Delta_{sc}}) \frac{\tan h(\beta\sqrt{\varepsilon_k^2 + (\Delta_{sc} + \Delta_{sdw})^2}/2)}{\sqrt{\varepsilon_k^2 + (\Delta_{sc} + \Delta_{sdw})^2}}$$

$$+ (1 - \frac{\Delta_{sdw}}{\Delta_{sc}}) \frac{\tan h(\sqrt{\varepsilon_k^2 + (\Delta_{sc} - \Delta_{sdw})^2}/2)}{\sqrt{\varepsilon_k^2 + (\Delta_{sc} - \Delta_{sdw})^2}} \} d\varepsilon. \tag{29}$$

Where $\lambda = VN(0)$.

Let I_1 and I_2 be defined by:

$$I_1 = \int_0^{\hbar\omega_F} \{ (1 + \frac{\Delta_{sdw}}{\Delta_{sc}}) \frac{\tan h(\beta\sqrt{\varepsilon_k^2 + (\Delta_{sc} + \Delta_{sdw})^2}/2)}{\sqrt{\varepsilon_k^2 + (\Delta_{sc} + \Delta_{sdw})^2}} \} d\varepsilon. \tag{30}$$

And

$$I_2 = \int_0^{\hbar\omega_F} \{1 - \frac{\Delta_{sdw}}{\Delta_{sc}}) \frac{\tan h(\beta\sqrt{\varepsilon_k^2 + (\Delta_{sc} - \Delta_{sdw})^2}/2)}{\sqrt{\varepsilon_k^2 + (\Delta_{sc} - \Delta_{sdw})^2}}\}. \quad (31)$$

As $T \to T_c$, $\Delta \to 0$ thus Equation (30) becomes:

$$I_1 = \int_0^{\hbar\omega_F} \{\frac{\tan h(\beta\sqrt{\varepsilon_k^2 + \Delta_{sdw}}/2)}{\sqrt{\varepsilon_k^2 + \Delta_{sdw}^2}}\}d\varepsilon. \quad (32)$$

Using Laplace transform, Equation (32) can be expressed as:

$$L_1 = \int_0^{\hbar\omega_F} \frac{\tan h(\beta\sqrt{\varepsilon_k^2 + \Delta_{sdw}^2}/2)}{\sqrt{\varepsilon_k^2 + \Delta_{sdw}^2}}d\varepsilon \quad (33)$$

$$-2\beta^3\Delta_{sdw}^2 \int_0^{\hbar\omega_F} d\varepsilon \sum_{n=-\infty}^{n=\infty} \frac{1}{(\pi(2n+1))^4(1+(\beta\varepsilon/\pi(2n+1))^2)}.$$

Using integration by parts, the first integral of Equation (33) can be integrated and obtain,

$$L_2 = \ln x - \ln(\pi/4\gamma), \quad (34)$$

where $\gamma = 1.78$ and is the Euler's constant.
    Finally we get:

$$L_2 = \ln(1.13\beta\hbar\omega_D). \quad (35)$$

Let the second part of Equation (35) be given by:

$$L_3 = -2\beta^3\Delta_{sdw}^2 \int_0^{\hbar\omega_F} d\varepsilon \sum_{n=-\infty}^{n=\infty} [\frac{1}{(\pi(2n+1))^4\{1+(\beta\varepsilon/\pi(2n+1))^2}. \quad (36)$$

From which we get:

$$L_3 = \frac{-4\beta^2\Delta_{sdw}^2}{\pi^3} \sum_{n=-\infty}^{n=\infty} \frac{1}{(2n+1)^3} \int_0^\infty \frac{1}{(1+y^2)^2}dy. \quad (37)$$

Employing the laws series and Zeta function, Equation (37) becomes:

$$L_3 = \frac{-7\Delta_{sdw}^2\beta^2\varsigma(3)}{8\pi^2}. \quad (38)$$

From the second part of Equation 30, we get:

$$I_4 = \int_0^{\hbar\omega} \lim_{\Delta \to 0} \frac{\Delta_{sdw}}{\Delta_{sc}} \frac{\tan h(\beta\sqrt{\varepsilon_k^2 + (\Delta_{sc} + \Delta_{sdw})^2}/2)}{\sqrt{\varepsilon_k^2 + (\Delta_{sc} + \Delta_{sdw})^2}}d\varepsilon. \quad (39)$$

Using L'Hopital's rule which is evaluated at the superconducting order parameter, Equation (39) becomes:

$$I_4 = \int_0^{\hbar\omega_F} \frac{\beta\Delta_{sdw}^2 \text{sech}^2(\sqrt{\varepsilon_k^2 + \Delta^2}sdw/2)}{2\sqrt{\varepsilon_k^2 + \Delta_{sdw}^2}}d\varepsilon. \quad (40)$$

Using trigonometric definitions Equation (40) becomes:

$$I_4 = [\int_0^{\hbar\omega_F} \{\frac{\beta\Delta_{sdw}^2}{2(\varepsilon_k^2 + \Delta_{sdw}^2)} - \frac{\beta\Delta_{sdw}^2\tan h(\beta\sqrt{\varepsilon_k^2 + \Delta_{sdw}^2}/2)}{2(\varepsilon_k^2 + \Delta_{sdw}^2)}\}d\varepsilon]. \quad (41)$$

The first part of Equation (41) can be evaluated using substitution method, such that:

$$Q = \int_0^{\hbar\omega_F} \frac{\beta\Delta_{sdw}^2}{2(\varepsilon_k^2 + \Delta_{sdw}^2)}d\varepsilon. \quad (42)$$

Let:

$$\varepsilon_k = \Delta_{sdw}\tan\gamma,$$

$$\Rightarrow d\varepsilon_k = \Delta_{sdw}\gamma\sec^2 d\gamma.$$

Thus, Equation (42) becomes:

$$Q = \frac{\beta\Delta_{sdw}}{4}\ln\{\frac{\hbar\omega_F + \Delta_{sdw}}{\hbar\omega_F - \Delta_{sdw}}\}. \quad (43)$$

Now, from Equations (41) and (43), we get:

$$L_4 = \frac{\beta\Delta_{sdw}}{4}\ln\{\frac{\hbar\omega_F + \Delta_{sdw}}{\hbar\omega_F - \Delta_{sdw}}\}$$

$$-\int_0^{\hbar\omega_F} \frac{\beta\Delta_{sdw}^2\tan h^2(\beta\sqrt{\varepsilon_k^2 + \Delta_{sdw}^2})}{2(\varepsilon_k^2 + \Delta_{sdw}^2)}d\varepsilon. \quad (44)$$

Using Equations (35), (38) and (41) in Equation (30), we get:

$$I_1 = \ln 1.13\beta\hbar\omega_F - \frac{7\Delta_{sdw}^2\beta^2\varsigma(3)}{8\pi^2} + \frac{\beta\Delta_{sdw}}{4}\ln\{\frac{\hbar\omega_F + \Delta_{sdw}}{\hbar\omega_F - \Delta_{sdw}}\}$$

$$-\int_0^{\hbar\omega_F} \frac{\beta\Delta_{sdw}^2\tan h^2(\beta\sqrt{\varepsilon_k^2 + \Delta_{sdw}^2}/2)}{2(\varepsilon_k^2 + \Delta_{sdw}^2)}d\varepsilon. \quad (45)$$

Equation (31) can be computed by employing similar method as for Equation (30) and obtain:

$$I_2 = \ln 1.13\beta\hbar\omega_F - \frac{7\Delta_{sdw}^2\varsigma(3)}{8\pi^2} + \frac{\beta\Delta_{sdw}}{4}\ln\{\frac{\hbar\omega_F + \Delta_{sdw}}{\hbar\omega_F - \Delta_{sdw}}\}$$

$$-\int_0^{\hbar\omega_F} \frac{\beta\Delta_{sdw}^2\tan h^2(\beta\sqrt{\varepsilon_k^2 + \Delta_{sdw}^2}/2)}{2(\varepsilon_k^2 + \Delta_{sdw}^2)}d\varepsilon. \quad (46)$$

Using Equations (45) and (46) in Equation (29) we get:

$$\frac{1}{\lambda} = \ln 1.13 \beta \hbar \omega_F - \frac{7\Delta_{sdw}^2 \beta^2 \varsigma(3)}{8\pi^2} + \frac{\beta \Delta_{sdw}}{4} \ln\{\frac{\hbar \omega_F + \Delta_{sdw}}{\hbar \omega_F - \Delta_{sdw}}\}$$

(47)

$$- \int_0^{\hbar \omega_F} \frac{\beta \Delta_{sdw}^2 \tanh^2(\beta \sqrt{\varepsilon_k^2 + \Delta_{sdw}^2}/2)}{2(\varepsilon_k^2 + \Delta_{sdw}^2)} d\varepsilon.$$

Neglecting the second and the fourth terms in Equation (47), we get:

$$\frac{1}{\lambda} = \ln 1.13 \beta \hbar \omega_F + \frac{\beta \Delta_{sdw}}{4} \ln\{\frac{\hbar \omega_F + \Delta_{sdw}}{\hbar \omega_F - \Delta_{sdw}}\}. \quad (48)$$

Let:

$$b = \frac{\beta}{4} \ln\{\frac{\hbar \omega_F + \Delta_{sdw}}{\hbar \omega_F - \Delta_{sdw}}\}. \quad (49)$$

Thus, using Equation (49) in Equation (48) and rearranging, the superconducting transition temperature (T_c) can be expressed as:

$$T_c = \frac{1.13 \hbar \omega_F}{k_B} \exp(-\frac{b\Delta_{sdw}}{\lambda}). \quad (50)$$

B. The order parameter of spin density wave (Δ_{sdw})

The order parameter of spin density wave can be expressed as:

$$\Delta_{sdw} = \frac{U}{\beta} \sum_k << C_{(k-q)\downarrow} C_{k\uparrow}^+ >>. \quad (51)$$

Substituting Equation (20) into Equation (51) we get:

$$\Delta_{sdw} = \frac{U\beta}{2} \sum_{n,k} \{\frac{\Delta_{sc} + \Delta_{sdw}}{(\pi(2n+1))^2 - \beta^2 \{\varepsilon_k^2 + (\Delta_{sc} + \Delta_{sdw})^2\}}$$

(52)

$$+ \frac{\Delta_{sdw} - \Delta_{sc}}{(\pi(2n+1))^2 + \beta^2 \{\Delta_{sdw} - \Delta_{sc})^2\}}.$$

$$\Delta_{sdw} = -\beta UN(0) \sum_n \int_0^{\hbar \omega_F} \{\frac{\Delta_{sc} + \Delta_{sdw}}{(\pi(2n+1))^2 + \beta^2 \{\varepsilon_k^2 + (\Delta_{sc} + \Delta_{sdw})^2\}}$$

(53)

$$+ \frac{\Delta_{sdw} - \Delta_{sc}}{(\pi(2n+1))^2 + \beta^2 \{\varepsilon_k^2 - (\Delta_{sc} + \Delta_{sdw})^2\}}\}d\varepsilon.$$

The sum may be changed into an integral by introducing the density of states, $N(0)$ as was done above and obtain:

$$\Delta_{sdw} = -\beta UN(0) \sum_n \int_0^{\hbar \omega_F} \{\frac{\Delta_{sc} + \Delta_{sdw}}{(\pi(2n+1))^2 + (\beta \varepsilon)^2}$$

(54)

$$+ \frac{\Delta_{sdw} - \Delta_{sc}}{(\pi(2n+1))^2 (\beta \varepsilon')^2}\}d\varepsilon.$$

Where:

$$\varepsilon^2 = \varepsilon_k^2 + (\Delta_{sc} + \Delta_{sdw})^2.$$

$$\varepsilon'^2 = \varepsilon_k^2 + (\Delta_{sdw} - \Delta_{sc})^2.$$

Now let us define:

$$\tanh(\beta \varepsilon / 2)/2\beta \varepsilon = \sum_n \frac{1}{(\pi(2n+1))^2 + (\beta \varepsilon)^2}. \quad (55)$$

$$\tanh(\beta \varepsilon / 2)/2\beta \varepsilon' = \sum_n \frac{1}{(\pi(2n+1))^2 + (\beta \varepsilon')^2}. \quad (56)$$

Using Equations (55) and (56) in Equation (54), we get:

$$\Delta_{sdw} = -\beta UN(0) \int_0^{\hbar \omega_F} \{(\Delta_{sc} + \Delta_{sdw}) \tanh(\beta \varepsilon / 2)/2\beta \varepsilon$$

$$+ (\Delta_{sdw} - \Delta_{sc}) \tanh(\beta \varepsilon'/2)/2\beta \varepsilon'\}d\varepsilon.$$

From which we get:

$$\frac{2}{\lambda'} = \int_0^{\hbar \omega_F} \{-(1+\frac{\Delta_{sc}}{\Delta_{sdw}})\frac{\tanh(\beta \sqrt{\{\varepsilon_k^2 + (\Delta_{sc} + \Delta_{sdw})^2\}/2})}{\sqrt{\varepsilon_k^2 + (\Delta_{sc} + \Delta_{sdw})^2}}$$

$$-(1-\frac{\Delta_{sc}}{\Delta_{sdw}})\frac{\tanh(\beta \sqrt{\{\varepsilon_k^2 + (\Delta_{sdw} - \Delta_{sc})^2\}/2})}{\sqrt{\varepsilon_k^2 + (\Delta_{sdw} - \Delta_{sc})^2}}\}d\varepsilon. \quad (58)$$

Where $\lambda' = UN(0)$

Let J_1 and J_2 be the integrals defined by:

$$J_1 = \int_0^{\hbar \omega_F} \{-(1+\frac{\Delta_{sc}}{\Delta_{sdw}})\frac{\tanh(\beta \sqrt{\{\varepsilon_k^2 + (\Delta_{sc} + \Delta_{sdw})^2\}/2})}{\sqrt{\varepsilon_k^2 + (\Delta_{sc} + \Delta_{sdw})^2}}\}d\varepsilon. \quad (59)$$

And:

$$J_2 = -\int_0^{\hbar \omega_F} \{(1-\frac{\Delta_{sc}}{\Delta_{sdw}})\frac{\tanh(\beta \sqrt{\{\varepsilon_k^2 + (\Delta_{sdw} - \Delta_{sc})^2\}/2})}{\sqrt{\varepsilon_k^2 + (\Delta_{sdw} - \Delta_{sc})^2}}\}d\varepsilon. \quad (60)$$

As $T \to T_{sdw}$, $\Delta_{sdw} \to 0$, then the first integral of Equation (59) becomes:

$$H_1 = -\int_0^{\hbar\omega_F} \left\{ \frac{\tan h(\beta\sqrt{\{\varepsilon_k^2 + \Delta_{sc}^2\}/2})}{\sqrt{\varepsilon_k^2 + \Delta_{sc}^2}} \right\} d\varepsilon. \quad (61)$$

Using Laplace transform, Equation (61) becomes:

$$H_1 = \int_0^{\hbar\omega_F} \frac{\tan h(\beta\sqrt{\varepsilon_k^2 + \Delta_{sc}^2}/2)}{\sqrt{\varepsilon_k^2 + \Delta_{sc}^2}} d\varepsilon -$$

$$2\beta^3\Delta_{sc}^2 \int_0^{\hbar\omega_F} d\varepsilon \sum_{n=-\infty}^{n=\infty} \frac{1}{(\pi(2n+1))^4\{1+(\frac{\beta\varepsilon}{\pi(2n+1)})^2\}}. \quad (62)$$

The first integral of Equation (62) can be integrated by using integration by parts and obtain:

$$H_2 = -\ln 1.13\beta\hbar\omega_F. \quad (63)$$

The second integral of Equation (62) can be integrated and obtain:

$$H_3 = \frac{4\beta^3\Delta_{sc}^2}{\pi^3} \sum_{n=-\infty}^{n=\infty} \frac{1}{(2n+1)^3} \int_0^\infty \frac{1}{(1+y^2)^2} dy. \quad (64)$$

Using the laws series and Zeta function, Equation (64) becomes:

$$H_3 = \frac{7\Delta_{sc}^2\beta^2\varsigma(3)}{8\pi^2}. \quad (65)$$

Furthermore, the second integral of Equation (59) can be solved as follows:

$$H_4 = \int_0^{\hbar\omega_F} \lim_{\Delta_{sdw}\to 0} \frac{\Delta_{sc}}{\Delta_{sdw}} \frac{\tan h(\beta\sqrt{\varepsilon_k^2 + (\Delta_{sc} + \Delta_{sdw})^2}/2)}{\sqrt{\varepsilon_k^2 + (\Delta_{sc} + \Delta_{sdw})^2}} d\varepsilon. \quad (66)$$

Using L'Hopital's rule, we get:

$$H_4 = -\int_0^{\hbar\omega_F} \frac{\beta\Delta_{sc}^2 \text{sech}^2(\beta\sqrt{\varepsilon_k^2 + \Delta_{sc}^2}/2)}{2(\varepsilon_k^2 + \Delta_{sc}^2)} d\varepsilon. \quad (67)$$

Using trigonometric definition Equation (67) becomes:

$$H_4 = -\left[\int_0^{\hbar\omega_F} \left\{ \frac{\beta\Delta_{sc}^2}{2(\varepsilon_k^2 + \Delta_{sc}^2)} - \frac{\beta\Delta_{sc}^2 \tanh^2(\beta\sqrt{\varepsilon_k^2 + \Delta_{sc}^2}/2)}{2(\varepsilon_k^2 + \Delta_{sc}^2)} \right\} d\varepsilon\right]. \quad (68)$$

The first part of the integral given in Equation (68) can be evaluated using substitution method as:

$$S = -\int_0^{\hbar\omega_F} \frac{\beta\Delta_{sc}^2}{2(\varepsilon_k^2 + \Delta_{sc}^2)} d\varepsilon.$$

Thus we get:

$$\therefore S = \frac{\beta\Delta_{sc}}{4}\ln\{\frac{\hbar\omega_F + \Delta_{sc}}{\hbar\omega_F - \Delta_{sc}}\}. \quad (69)$$

Using Equation (69) in Equation (68), we get:

$$H_4 = \frac{\beta\Delta_{sc}}{4}\ln\{\frac{\hbar\omega_F + \Delta_{sc}}{\hbar\omega_F - \Delta_{sc}}\} -$$

$$\int_0^{\hbar\omega_F} \frac{\beta\Delta_{sc}^2 \tan h^2(\beta\sqrt{\varepsilon_k^2 + \Delta_{sc}^2}/2)}{2(\varepsilon_k^2 + \Delta_{sc}^2)} d\varepsilon. \quad (70)$$

Finally, using Equations (63), (65), (70), and (59) becomes:

$$J_1 = -\ln 1.13\beta\hbar\omega_F + \frac{7\Delta_{sc}^2\beta^2\varsigma(3)}{8\pi^2} - \frac{\beta\Delta_{sc}}{4}\ln\{\frac{\hbar\omega_F + \Delta_{sc}}{\hbar\omega_F - \Delta_{sc}}\}$$

$$+ \int_0^{\hbar\omega_F} \left\{ \frac{\beta\Delta_{sc}^2 \tan h^2(\beta\sqrt{\varepsilon_k^2 + \Delta_{sc}^2}/2)}{2(\varepsilon_k^2 + \Delta_{sc}^2)} \right\} d\varepsilon. \quad (71)$$

Furthermore, Equation (60) can be computed by employing similar method as for Equation (59) and obtain:

$$J_2 = -\ln 1.13\beta\hbar\omega_F + \frac{7\Delta_{sc}^2\beta^2\varsigma(3)}{8\pi^2} - \frac{\beta\Delta_{sc}}{4}\ln\{\frac{\hbar\omega_F + \Delta_{sc}}{\hbar\omega_F - \Delta_{sc}}\}$$

$$+ \int_0^{\hbar\omega_F} \frac{\beta\Delta_{sc}^2 \tan h^2(\beta\sqrt{\varepsilon_k^2 + \Delta_{sc}^2}/2)}{2(\varepsilon_k^2 + \Delta_{sc}^2)} d\varepsilon. \quad (72)$$

Now, using Equations (71) and (72) in Equation (58) we get:

$$-\frac{1}{\lambda'} = \ln 1.13\beta\hbar\omega_F - \frac{7\Delta_{sc}^2\beta^2\varsigma(3)}{8\pi^2} + \frac{\beta\Delta_{sc}}{4}\ln(\frac{\hbar\omega_F + \Delta_{sc}}{\hbar\omega_F - \Delta_{sc}})$$

$$+ \int_0^{\hbar\omega_F} \left\{ \frac{\beta\Delta_{sc}^2 \tan h^2(\beta\sqrt{\varepsilon_k^2 + \Delta_{sc}^2}/2)}{2(\varepsilon_k^2 + \Delta_{sc}^2)} \right\} d\varepsilon. \quad (73)$$

Neglecting the second and the fourth terms in Equation (73), we get:

$$-\frac{1}{\lambda'} = \ln 1.13\beta\hbar\omega_F + \frac{\beta\Delta_{sc}}{4}\ln(\frac{\hbar\omega_F + \Delta_{sc}}{\hbar\omega_F - \Delta_{sc}}). \quad (74)$$

Let:

$$\eta = \frac{\beta}{4}\ln(\frac{\hbar\omega_F + \Delta_{sc}}{\hbar\omega_F - \Delta_{sc}}). \quad (75)$$

Therefore, Equation (74) becomes:

$$-\frac{1}{\lambda'} = \ln 1.13\beta\hbar\omega_F + \eta\Delta_{sc}. \quad (76)$$

From which we get:

$$T_{sdw} = \frac{1.13\hbar\omega_F}{k_B}\exp(\frac{1}{\lambda'} + \eta\Delta_{sc}). \quad (77)$$

C. Order parameter in pure superconducting region

In pure superconducting region, $\Delta_{sdw} \to 0$.

Thus we get:

$$\frac{1}{\lambda} = \int_0^{\hbar\omega_F} (\frac{\tanh^2(\beta\sqrt{\varepsilon_k^2 + \Delta_{sc}^2}/2)}{\sqrt{\varepsilon_k^2 + \Delta_{sc}^2}})d\varepsilon. \quad (78)$$

Using Laplace transform, Equation 78 can be expressed as:

$$I_1' = \int_0^{\hbar\omega} \frac{\tanh^2(\beta\sqrt{\varepsilon_k^2 + \Delta_{sc}^2}/2)}{\sqrt{\varepsilon_k^2 + \Delta_{sc}^2}}d\varepsilon$$

$$-\int_0^{\hbar\omega} \Delta_{sc}^2 d\varepsilon \frac{2}{\beta} \sum_{n=-\infty}^{n=\infty} \frac{1}{\{(\pi(2n+1)\beta^{-1})^2 + \varepsilon_k^2\}^2}. \quad (79)$$

The first part of Equation (79) can be integrated by parts. Let:

$$I_1'' = \ln 1.13\beta\hbar\omega_F. \quad (80)$$

From the second part of Equation (79), we get:

$$I_1'' = -\frac{4\beta^2\Delta_{sc}^2}{\pi^3} \sum_{n=-\infty}^{n=\infty} \frac{1}{(2n+1)^3} \int_0^\infty \frac{1}{((1+y^2)^2)}dy. \quad (81)$$

Using the laws series and Zeta function, we get:

$$I_1'' = -\frac{7\Delta_{sc}^2\beta^2\varsigma(3)}{8\pi^2}. \quad (82)$$

Finally, Equation (78) can be expressed as:

$$\frac{1}{\lambda} = \ln 1.13\beta\hbar\omega_F - \frac{7\Delta_{sc}^2\beta^2\varsigma(3)}{8\pi^2}. \quad (83)$$

In pure superconducting region Equation (50) can be reduced to the well-known BCS form. That is:

$$T_c = \frac{1.13\hbar\omega_F}{k_B}\exp(-\frac{1}{\lambda}). \quad$$

Rearranging Equation (84), we get:

$$\frac{1}{\lambda} = \ln 1.13\frac{\hbar\omega_F}{k_BT_c}. \quad (85)$$

From Equations (83) and (84), we get:

$$\ln 1.13\frac{\hbar\omega_F}{k_BT_c} = \ln 1.13\beta\hbar\omega_F - \frac{7\Delta_{sc}^2\beta^2\varsigma(3)}{8\pi^2}. \quad (86)$$

Equation (88) can be rewritten as:

$$\ln\{1 - (1 - \frac{T}{T_c})\} = -\frac{7\Delta_{sc}^2\beta^2\varsigma(3)}{8\pi^2}. \quad (87)$$

But:

$$\ln\{1 - (1 - y)\} = -(1 - y) - \frac{(1-y)^2}{2}. \quad (88)$$

Now using Equation (88) in Equation (87), we get:

$$1 - \frac{T}{T_c} \approx \frac{7\Delta_{sc}^2\beta^2\varsigma(3)}{8\pi^2}. \quad (89)$$

From which we get:

$$\Delta_{sc}(T) = 3.06k_BT\sqrt{1 - \frac{T}{T_c}}. \quad (90)$$

D. Order parameter in pure spin density wave region

In pure spin density wave region, $\Delta_{sc} \to 0$. Thus we get:

$$\frac{1}{\lambda'} = -\int_0^{\hbar\omega_F} \frac{\tanh(\beta\sqrt{\varepsilon_k^2 + \Delta_{sdw}^2}/2)}{\sqrt{\varepsilon_k^2 + \Delta_{sdw}^2}}d\varepsilon. \quad (91)$$

Using Laplace transform, Equation (91) can be expressed as:

$$J_1' = \int_0^{\hbar\omega_F} \frac{\tanh(\beta\sqrt{\varepsilon_k^2 + \Delta_{sdw}^2}/2)}{\sqrt{\varepsilon_k^2 + \Delta_{sdw}^2}}d\varepsilon - $$
$$\int_0^{\hbar\omega_F} \Delta_{sdw}^2 d\varepsilon \frac{2}{\beta} \sum_{n=-\infty}^{n=\infty} \frac{1}{(\pi(2n+1)\beta^{-1})^2 + \varepsilon_k^2}. \quad (92)$$

The first integral of Equation (92) can be integrated by parts and obtain:

$$J_1'' = -\ln 1.13\beta\hbar\omega_F. \quad (93)$$

From the second part of Equation (92), we get:

$$J_1^{''} = -2\beta^3 \Delta_{sdw}^2 \int_0^{\hbar\omega_F} d\varepsilon \sum_{n=-\infty}^{n=\infty} \frac{1}{(\pi(2n+1))^4 \{1+(\frac{\beta\varepsilon}{\pi(2n+1)})^2\}}. \quad (94)$$

From which we get:

$$J_1^{'''} = -\frac{4\beta^2\Delta_{sdw}^2}{\pi^3} \sum_{n=-\infty}^{n=\infty} \frac{1}{(2n+1)^3} \int_0^\infty \frac{1}{((1+y^2)^2} dy. $$

Using the laws series and Zeta function, we get:

$$J_1^{'''} = -\frac{7\Delta_{sdw}^2\beta^2\varsigma(3)}{8\pi^2}. \quad (95)$$

Hence, using Equations (93) and (95), in Equation (91), we get:

$$\frac{1}{\lambda'} = \ln 1.13\beta\hbar\omega_F - \frac{7\Delta_{sdw}^2\beta^2\varsigma(3)}{8\pi^2}. \quad (96)$$

For $\Delta_{sc} = 0$, Equation (77) becomes:

$$\frac{1}{\lambda'} = \ln 1.13\frac{\hbar\omega_F}{k_B T_{sdw}}. \quad (97)$$

Now from Equations (96) and (97), we get:

$$\ln 1.13\frac{\hbar\omega_F}{K_B T_{sdw}} = \ln 1.13\beta\hbar\omega_F - \frac{7\Delta_{sdw}\beta^2\varsigma(3)}{8\pi^2}$$

$$\therefore \ln(1-(1+\frac{T}{T_{sdw}})) = -\frac{7\Delta_{sdw}^2\beta^2\varsigma(3)}{8\pi^2} \quad (98)$$

Using the relation:

$$\ln(1-(1+y)) = -(1+y) - \frac{(1+y)^2}{2}. \quad (99)$$

Using Equation (99) in Equation (98), we get:

$$\Delta_{sdw}(T) = 3.06 k_B T_{sdw} \sqrt{1+\frac{T}{T_{sdw}}}. \quad (100)$$

III. RESULTS AND DISCUSSION

In this work, we developed the equation of motion by employing quantum field theory Green function formalism and obtained Equation (90), which yields the relationship between the superconducting order parameter (Δ_{sc}) and the

superconducting transition temperature (T_c) for a superconductor and Equation 100 yields the relationship between the spin density wave order parameter (Δ_{sc}) and the spin density wave transition temperature (T_{sdw}).

The expression we obtained for a pure superconductor is in agreement with the BCS theory in the absence of spin density wave order parameter ($\Delta_{sdw} = 0$).

The superconductivity order parameter, which is the measure of pairing energy decreases with increasing temperature and vanishes at the transition temperature (T_c).

Using the experimental value of T_c for BaFe$_{2-x}$Co$_x$As$_2$, we plotted the transition temperature T_c vs. superconducting order parameter (Δ_{sc}) as indicated in Figure 1.
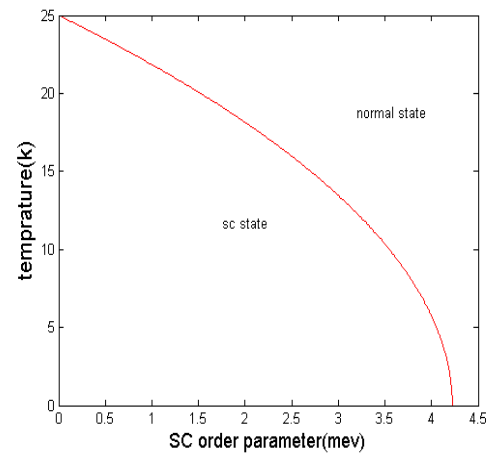

FIGURE 1. Superconducting transition temperature (T_c) versus superconducting order parameter (Δ_{sc}).

Furthermore, the spin density wave transition temperature (T_{sdw}) versus spin density wave order parameter (Δ_{sdw}) of BaFe$_{2-x}$Co$_x$As$_2$ is plotted as shown in Figure 2.

FIGURE 2. Spin density wave transition temperature (T_{sdw}) versus spin density wave order parameter (Δ_{sdw}).

Now, by combining Figures 1 and 2, we get a region in which both spin density wave and superconductivity coexist as shown in Figure 3. As is indicated in Figure 3, our finding is in agreement with the experimental observations [11].

IV. CONCLUSION

In this paper, we developed model hamiltonian and by employing quantum field theory Green function formalism, we have analyzed theoretically the coexistence of spin density wave and superconductivity in $BaFe_{2-x}Co_xAs_2$. By plotting phase diagrams we obtained the possible region of coexistence of spin density wave and superconductivity in $BaFe_{2-x}Co_xAs_2$. The result we obtained is in agreement with the experimental observations [11].
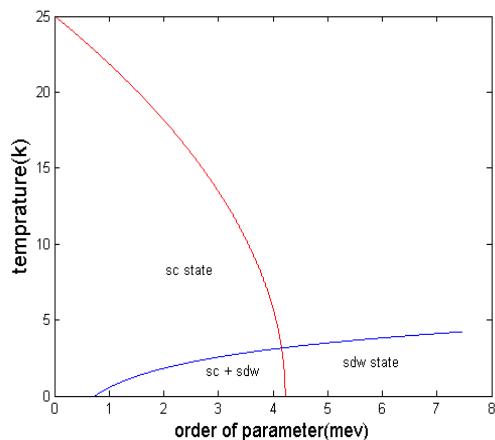

FIGURE 3. Coexistence of spin density wave and superconductivity in superconducting $BaFe_{2-x}Co_xAs_2$.

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