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Coexistence of Spin Density Wave (SDW) and Superconductivity in $Ba_{1-x}K_xFe_2As_2$

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Abstract

With the use of a model Hamiltonian and retarded double time green's function formalism, we obtain mathematical expressions for spin density wave and superconductivity parameters. The model reveals a distinct possibility of the coexistence of magnetic phase and superconductivity, which are two usually irreconcilable cooperative phenomena. The work is motivated by the recent experimental evidences of coexistence of spin density wave and superconductivity in a number of FeAs-based superconductors. The theoretical results are then applied to show the coexistence of spin density wave and superconductivity in iron pnictide compound $Ba_{1-x}K_xFe_2As_2$ ($0.2 \le x < 0.4$).

Keywords

Retarded Double Time Green's Function Formalism, Spin Singlet and Triplet State, Spin Density Wave and Superconducting

1. Introduction

The interplay between superconductivity and magnetism has been an interesting topic in condensed mater physics which has been considered until very recently hostile and incompatible. Since the discovery of superconductivity in quaternary pnictide-oxides with critical temperatures (T_C) up to 55 K a lot of tremendous interest has been generated in the study of coexistence of these two cooperative phenomena of superconductivity and magnetism. After first reports on superconductivity in undoped LaNiPO [1] [2] below 5 K, shortly after this discovery the breakthrough was a T_C of 26 K in the F-doped arsenide $LaO_{1-x}F_xFeAs$ system [3].

In addition to this several groups reported an increase of T_C values by replacing La with smaller-size rare-earth ions like $CeO_{1-x}F_xFeAs$ [4], and samarium-arsenide oxides $Sm(O_{1-x}F_x)FeAs$ with a critical temperature T_C of 55 K [5] [6]. The iron based superconductors promise interesting applications. While the interplay of superconductivity and magnetism, as well as their mechanisms remains the issues of active debates and studies, one thing in FeSC riddle is clear that it is the complex multi-band electronic structure of these compounds that determine their rich and puzzling properties. What is important and captivating is that this complexity seems to play a positive role in the struggle for understanding the FeSC physics and also for search of the materials with higher T_C [7].

The FeSC is quite promising for applications. Having much higher Hc than cuprates and high isotropic critical currents [8] they are attractive for electrical power and magnet applications, while the coexistence of magnetism and superconductivity makes them interesting for spintronics [9]. All the compounds share similar electronic band structure in which the electronic states at the Fermi level are occupied predominantly by the Fe 3d electrons [7].

By combining transport, X-ray and neutron diffraction experiment studies, the first member of a new family of iron pnictide superconductors $(Ba_{1-x}K_x)Fe_2As_2$ with the $ThCr_2Si_2$-type structure was discovered a bulk superconductor with $T_C = 38$ K and both the SDW and the superconducting orders coexist in the $(Ba_{1-x}K_x)Fe_2As_2$ $(0.2 \leq x < 0.4)$. The structural and electronic properties of the parent compound $BaFe_2As_2$ are closely related to LaFeAsO. The induced superconductivity by hole doping is found to have a significantly higher TC in comparison with hole doped LaFeAsO. In contrast to previously stated opinions, the results prove that hole doping is definitely a possible pathway to induce high-T_C superconductivity, at least in the oxygen-free compounds [10].

The above exciting discovery stimulated a lot of interest in the study of coexistence of superconductivity and magnetism. The proximity of the magnetic and superconducting (SC) phases suggests a close relationship between the two phenomena. 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. Besides, other experimental and theoretical findings, especially the antiferromagnetic ground state and the SDW anomaly of LaFeAsO strongly suggest that the pairing mechanism of the electrons is likely to be connected with spin fluctuations, as it has been assumed for the cuprates [10].

Triplet superconductivity appears provided that we have coexistence of singlet superconductivity and SDW. In many high T_{sc} superconductors, superconducting mechanism is attributed to strong coulomb interactions of the electrons in the system, which can also be the cause for the appearance of SDW state. This suggests the existence of competition between the two states [11]. The properties of the unconventional triplet superconductivity and SDW with an emphasis on the analysis of their order parameter were reviewed.

Research on superconducting iron arsenides has largely focused on ternary compounds with the $ThCr_2Si_2$-type structure, rather than arsenide oxides (LaFeAsO derivatives) [12]. This is because single-phase samples and also large single crystals of the ternary compounds are much easier to obtain. Partial replacement of barium for potassium (hole doping) induced superconductivity at 38 K in $(Ba_{0.6}K_{0.4})Fe_2As_2$, [13].

The relation between the spin-density-wave (SDW) and superconducting order is a central topic in current research on the superconducting iron pnictide based high TC superconductors. So, in this paper, we start with a model Hamiltonian which incorporates not only terms of the BCS but also by assuming the pairing interaction is due to spin fluctuations for iron pnictide superconductors $Ba_{1-x}K_xFe_2As_2$, to examine the coexistence of spin density wave and superconductivity.

2. Model Hamiltonian of the System

The purpose of this work is to study theoretically the co-existence of spin density wave and superconductivity properties in the compound $Ba_{1-x}K_xFe_2As_2$ in general and to find expression for transition temperature and order parameter in particular. For this purpose, we tried to find the mathematical expression for the superconducting critical temperature (T_C), superconducting order parameter (Δ_{sc}) the magnetic order parameter (M) and SDW transition temperature (T_{SDW}). Within the framework of the BCS model, the model of the Hamiltonian for coexistence SDW and superconductivity in the compound can be express as:

$$H = \sum_{p\sigma} \epsilon_p \hat{a}^{\dagger}_{p\sigma} \hat{a}_{p\sigma} + M \sum_{p} \left(\hat{a}^{\dagger}_{p+q\uparrow} \hat{a}_{-p\downarrow} + \hat{a}^{\dagger}_{-p\downarrow} \hat{a}_{p+q\uparrow} \right) + \Delta_{SC} \sum_{p} \left(\hat{a}^{\dagger}_{p\uparrow} \hat{a}^{\dagger}_{-p\downarrow} + \hat{a}_{-p\downarrow} \hat{a}_{p\uparrow} \right) \quad (1)$$

where $\left(\hat{a}^{\dagger}_{p\sigma} \hat{a}_{p\sigma} \right)$ are the creation (annihilation) operators of an electron having the wave number p and spin σ. Whereas (Δ_{SC}) superconducting order parameter and (M) SDW order parameters. The Hamiltonian in (1) will be used to determine the equations of motion in terms of the Green function.

2.1. Coupling of SDW and Superconducting Order Parameters

The Double time dependent Green's function equal to the change of the average value of some dynamic quantity by the time t and useful because they can be used to describe the effect of retarded interactions and all quantities of physical interest can be derived from them. To get the equation of motion we use the double-time temperature dependent retarded Green function is given by Zubarev [14]:

$$G_r(t-t') \equiv \langle\langle \hat{A}(t); \hat{B}(t') \rangle\rangle$$
$$\text{or } G_r(t,t') = -i\theta(t-t') \langle [\hat{A}(t), \hat{B}(t')] \rangle \tag{2}$$

where $\hat{A}$ and $\hat{B}$ are Heisenberg operators and $\theta(t-t')$ is the Heaviside step function. Now, using Dirac delta function and Heisenberg operators, we can write as:

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

The Fourier transformation $G_r(\omega)$ is given by

$$G_r(t-t') = \int G_r(\omega) \exp[-i\omega(t-t')] \mathrm{d}\omega. \tag{3}$$

Taking the Fourier transform we get:

$$\omega G_r(\omega) = \langle [\hat{A}(t), \hat{B}(t')] \rangle_\omega + \langle\langle [\hat{A}(t), H], \hat{B}(t') \rangle\rangle_\omega. \tag{4}$$

From (4), it follows that

$$\omega \langle\langle \hat{a}^\dagger_{\kappa\uparrow}, \hat{a}^\dagger_{-\kappa\downarrow} \rangle\rangle = \langle\langle [\hat{a}^\dagger_{\kappa\uparrow}, H], \hat{a}^\dagger_{-\kappa\downarrow} \rangle\rangle \tag{5}$$

where the anti-commutation relation,

$$\{\hat{a}_{\kappa\sigma}, \hat{a}^\dagger_{k'\sigma'}\} = \delta_{kk'}\delta_{\sigma\sigma'} \tag{6}$$

has been used. To derive an expression for $\langle\langle \hat{a}^\dagger_{\kappa\uparrow}, \hat{a}^\dagger_{-\kappa\downarrow} \rangle\rangle$, we have calculate the commutator $[\hat{a}^\dagger_{\kappa\uparrow}, H]$, using (1) and using the identities and

$$[A, BC] = \{A, B\}C - B\{A, C\} \quad \text{and} \quad [AB, C] = A\{B, C\} - \{A, C\}B. \tag{7}$$

Solving the commutator in Equation (5) by using the Hamiltonian in e Equation (1), we get

$$\left[\hat{a}^\dagger_{\kappa\uparrow}, \sum_{p\sigma}\epsilon_p \hat{a}^\dagger_{p\sigma}\hat{a}_{p\sigma}\right] = \sum_{p\sigma}\epsilon_p [\hat{a}^\dagger_{\kappa\uparrow}, \hat{a}^\dagger_{p\sigma}\hat{a}_{p\sigma}] = \sum_{p\sigma}\epsilon_p \left(\{\hat{a}^\dagger_{\kappa\uparrow}, \hat{a}^\dagger_{p\sigma}\}\hat{a}_{p\sigma} - \hat{a}^\dagger_{p\sigma}\{\hat{a}^\dagger_{\kappa\uparrow}, \hat{a}_{p\sigma}\}\right)$$

$$\left[\hat{a}^\dagger_{\kappa\uparrow}, \sum_{p\sigma}\epsilon_p \hat{a}^\dagger_{p\sigma}\hat{a}_{p\sigma}\right] = -\epsilon_\kappa \hat{a}^\dagger_{\kappa\uparrow}. \tag{8a}$$

After some lengthy but straightforward calculations; we arrive at the following results:

$$\left[\hat{a}^\dagger_{\kappa\uparrow}, M\sum_{\kappa}\left(\hat{a}^\dagger_{\kappa+q\uparrow}\hat{a}_{-\kappa\downarrow} + \hat{a}^\dagger_{-\kappa\downarrow}\hat{a}_{\kappa+q\uparrow}\right)\right] = -M\hat{a}^\dagger_{\kappa-q\downarrow} \tag{8b}$$

$$\left[\hat{a}^\dagger_{\kappa\uparrow}, \Delta_{\mathrm{SC}}\sum_{p}\left(\hat{a}^\dagger_{p\uparrow}\hat{a}^\dagger_{-p\downarrow} + \hat{a}_{-p\downarrow}\hat{a}_{p\uparrow}\right)\right] = -\Delta_{\mathrm{SC}}\hat{a}_{-k\downarrow}. \tag{8c}$$

Substituting (8) in to (5), we get

$$\omega\langle\langle \hat{a}^\dagger_{\kappa\uparrow}, \hat{a}^\dagger_{-\kappa\downarrow} \rangle\rangle = -\epsilon_\kappa \langle\langle \hat{a}^\dagger_{\kappa\uparrow}, \hat{a}^\dagger_{-\kappa\downarrow} \rangle\rangle - M\langle\langle \hat{a}^\dagger_{\kappa-q\downarrow}, \hat{a}^\dagger_{-\kappa\downarrow} \rangle\rangle - \Delta_{\mathrm{SC}}\langle\langle \hat{a}_{-k\downarrow}, \hat{a}^\dagger_{-\kappa\downarrow} \rangle\rangle$$

$$(\omega + \epsilon_\kappa)\langle\langle \hat{a}^\dagger_{\kappa\uparrow}, \hat{a}^\dagger_{-\kappa\downarrow} \rangle\rangle = -M\langle\langle \hat{a}^\dagger_{\kappa-q\downarrow}, \hat{a}^\dagger_{-\kappa\downarrow} \rangle\rangle - \Delta_{\mathrm{SC}}\langle\langle \hat{a}_{-k\downarrow}, \hat{a}^\dagger_{-\kappa\downarrow} \rangle\rangle. \tag{9}$$

The equation of motion for the correlation $\left\langle\left\langle \hat{a}^{\dagger}_{\kappa-q\downarrow}, \hat{a}^{\dagger}_{-\kappa\downarrow} \right\rangle\right\rangle$ in (9) can be described as:

$$\omega\left\langle\left\langle \hat{a}^{\dagger}_{\kappa-q\downarrow}, \hat{a}^{\dagger}_{-\kappa\downarrow} \right\rangle\right\rangle = \delta_{kk'} + \left\langle\left\langle \left[\hat{a}^{\dagger}_{\kappa-q\downarrow}, H\right], \hat{a}^{\dagger}_{-\kappa\downarrow} \right\rangle\right\rangle$$

$$\omega\left\langle\left\langle \hat{a}^{\dagger}_{\kappa-q\downarrow}, \hat{a}^{\dagger}_{-\kappa\downarrow} \right\rangle\right\rangle = \left\langle\left\langle \left[\hat{a}^{\dagger}_{\kappa-q\downarrow}, H\right], \hat{a}^{\dagger}_{-\kappa\downarrow} \right\rangle\right\rangle. \tag{10}$$

Evaluating the commutator in Equation (10) using Hamiltonian:

$$\left[\hat{a}^{\dagger}_{\kappa-q\downarrow}, \sum_{p\sigma}\epsilon_p \hat{a}^{\dagger}_{p\sigma}\hat{a}_{p\sigma}\right] = \sum_{p\sigma}\epsilon_p\left[\hat{a}^{\dagger}_{\kappa-q\downarrow}, \hat{a}^{\dagger}_{p\sigma}\hat{a}_{p\sigma}\right]$$

$$= \sum_{p\sigma}\epsilon_p\left(\left\{\hat{a}^{\dagger}_{\kappa-q\downarrow}, \hat{a}^{\dagger}_{p\sigma}\right\}\hat{a}_{p\sigma} - \hat{a}^{\dagger}_{p\sigma}\left\{\hat{a}^{\dagger}_{\kappa-q\downarrow}, \hat{a}_{p\sigma}\right\}\right)$$

$$\left[\hat{a}^{\dagger}_{\kappa-q\downarrow}, \sum_{p\sigma}\epsilon_p \hat{a}^{\dagger}_{p\sigma}\hat{a}_{p\sigma}\right] = -\epsilon_{\kappa-q}\hat{a}^{\dagger}_{\kappa-q\downarrow}. \tag{11a}$$

After some lengthy but straightforward calculations; we arrive at the following results:

$$\left[\hat{a}^{\dagger}_{\kappa-q\downarrow}, M\sum_{\kappa}\left(\hat{a}^{\dagger}_{\kappa+q\uparrow}\hat{a}_{-\kappa\downarrow} + \hat{a}^{\dagger}_{-\kappa\downarrow}\hat{a}_{\kappa+q\uparrow}\right)\right] = -M\hat{a}^{\dagger}_{\kappa\uparrow} \tag{11b}$$

$$\left[\hat{a}^{\dagger}_{\kappa-q\downarrow}, \Delta_{\mathrm{SC}}\sum_{p}\left(\hat{a}^{\dagger}_{p\uparrow}\hat{a}^{\dagger}_{-p\downarrow} + \hat{a}_{-p\downarrow}\hat{a}_{p\uparrow}\right)\right] = \Delta_{\mathrm{SC}}\hat{a}_{-k+q\downarrow}. \tag{11c}$$

Substituting (11) in to (10), we get

$$\omega\left\langle\left\langle \hat{a}^{\dagger}_{\kappa-q\downarrow}, \hat{a}^{\dagger}_{-\kappa\downarrow} \right\rangle\right\rangle = -\square_{\kappa-q}\left\langle\left\langle \hat{a}^{\dagger}_{\kappa-q\downarrow}, \hat{a}^{\dagger}_{-\kappa\downarrow} \right\rangle\right\rangle - M\left\langle\left\langle \hat{a}^{\dagger}_{\kappa\uparrow}, \hat{a}^{\dagger}_{-\kappa\downarrow} \right\rangle\right\rangle$$

$$+ \Delta_{\mathrm{SC}}\left\langle\left\langle \hat{a}_{-k+q\downarrow}, \hat{a}^{\dagger}_{-\kappa\downarrow} \right\rangle\right\rangle$$

$$\left(\omega+\epsilon_{\kappa-q}\right)\left\langle\left\langle \hat{a}^{\dagger}_{\kappa-q\downarrow}, \hat{a}^{\dagger}_{-\kappa\downarrow} \right\rangle\right\rangle = -M\left\langle\left\langle \hat{a}^{\dagger}_{\kappa\uparrow}, \hat{a}^{\dagger}_{-\kappa\downarrow} \right\rangle\right\rangle + \Delta_{\mathrm{SC}}\left\langle\left\langle \hat{a}_{-k+q\downarrow}, \hat{a}^{\dagger}_{-\kappa\downarrow} \right\rangle\right\rangle. \tag{12}$$

Similarly as we did in the above the equation of motion for the correlation $\left\langle\left\langle \hat{a}_{-\kappa+q\uparrow}, \hat{a}^{\dagger}_{-\kappa\downarrow} \right\rangle\right\rangle$ and $\left\langle\left\langle \hat{a}_{-\kappa\downarrow}, \hat{a}^{\dagger}_{-\kappa\downarrow} \right\rangle\right\rangle$ is given by:

$$\omega\left\langle\left\langle \hat{a}_{-\kappa+q\uparrow}, \hat{a}^{\dagger}_{-\kappa\downarrow} \right\rangle\right\rangle = \epsilon_{-\kappa+q}\left\langle\left\langle \hat{a}_{-\kappa+q\uparrow}, \hat{a}^{\dagger}_{-\kappa\downarrow} \right\rangle\right\rangle + M\left\langle\left\langle \hat{a}_{-\kappa\downarrow}, \hat{a}^{\dagger}_{-\kappa\downarrow} \right\rangle\right\rangle + \Delta_{\mathrm{SC}}\left\langle\left\langle \hat{a}^{\dagger}_{\kappa-q\downarrow}, \hat{a}^{\dagger}_{-\kappa\downarrow} \right\rangle\right\rangle$$

$$\left(\omega-\epsilon_{-\kappa+q}\right)\left\langle\left\langle \hat{a}_{-\kappa+q\uparrow}, \hat{a}^{\dagger}_{-\kappa\downarrow} \right\rangle\right\rangle = M\left\langle\left\langle \hat{a}_{-\kappa\downarrow}, \hat{a}^{\dagger}_{-\kappa\downarrow} \right\rangle\right\rangle + \Delta_{\mathrm{SC}}\left\langle\left\langle \hat{a}^{\dagger}_{\kappa-q\downarrow}, \hat{a}^{\dagger}_{-\kappa\downarrow} \right\rangle\right\rangle \tag{13}$$

and

$$\left(\omega-\epsilon_{-\kappa}\right)\left\langle\left\langle \hat{a}_{-\kappa\downarrow}, \hat{a}^{\dagger}_{-\kappa\downarrow} \right\rangle\right\rangle = 1 + M\left\langle\left\langle \hat{a}_{-\kappa+q\uparrow}, \hat{a}^{\dagger}_{-\kappa\downarrow} \right\rangle\right\rangle - \Delta_{\mathrm{SC}}\left\langle\left\langle \hat{a}^{\dagger}_{\kappa\uparrow}, \hat{a}^{\dagger}_{-\kappa\downarrow} \right\rangle\right\rangle. \tag{14}$$

From Equation (12), we obtain:

$$\left\langle\left\langle \hat{a}^{\dagger}_{\kappa-q\downarrow}, \hat{a}^{\dagger}_{-\kappa\downarrow} \right\rangle\right\rangle = \frac{-M\left\langle\left\langle \hat{a}^{\dagger}_{\kappa\uparrow}, \hat{a}^{\dagger}_{-\kappa\downarrow} \right\rangle\right\rangle}{\left(\omega+\epsilon_{\kappa-q}\right)} + \frac{\Delta_{\mathrm{SC}}\left\langle\left\langle \hat{a}_{-k+q\downarrow}, \hat{a}^{\dagger}_{-\kappa\downarrow} \right\rangle\right\rangle}{\left(\omega+\epsilon_{\kappa-q}\right)}. \tag{15}$$

And from Equation (14):

$$\left\langle\left\langle \hat{a}_{-\kappa\downarrow}, \hat{a}^{\dagger}_{-\kappa\downarrow} \right\rangle\right\rangle = \frac{1}{\left(\omega-\epsilon_{-\kappa}\right)} + \frac{M\left\langle\left\langle \hat{a}_{-\kappa+q\uparrow}, \hat{a}^{\dagger}_{-\kappa\downarrow} \right\rangle\right\rangle}{\left(\omega-\epsilon_{-\kappa}\right)} - \frac{\Delta_{\mathrm{SC}}\left\langle\left\langle \hat{a}^{\dagger}_{\kappa\uparrow}, \hat{a}^{\dagger}_{-\kappa\downarrow} \right\rangle\right\rangle}{\left(\omega-\epsilon_{-\kappa}\right)}. \tag{16}$$

Plugging Equations (15) and (16) in (9), yields:

$$\left(\omega+\epsilon_\kappa-\frac{M^2}{\left(\omega+\epsilon_{\kappa-q}\right)}-\frac{\Delta_{\mathrm{SC}}^2}{\left(\omega-\epsilon_{-\kappa}\right)}\right)\left\langle\left\langle\hat{a}_{\kappa\uparrow}^\dagger,\hat{a}_{-\kappa\downarrow}^\dagger\right\rangle\right\rangle$$
$$=-\frac{\Delta_{\mathrm{SC}}}{\left(\omega-\epsilon_{-\kappa}\right)}-\left(\frac{M\Delta_{\mathrm{SC}}}{\left(\omega+\epsilon_{\kappa-q}\right)}+\frac{M\Delta_{\mathrm{SC}}}{\left(\omega-\epsilon_{-\kappa}\right)}\right)\left\langle\left\langle\hat{a}_{-k+q\downarrow},\hat{a}_{-\kappa\downarrow}^\dagger\right\rangle\right\rangle. \tag{17}$$

And insert Equations (15) and (16) in (13), we have:

$$\left(\left(\omega-\epsilon_{-\kappa+q}\right)-\frac{M^2}{\left(\omega-\epsilon_{-\kappa}\right)}-\frac{\Delta_{\mathrm{SC}}^2}{\left(\omega+\epsilon_{\kappa-q}\right)}\right)\left\langle\left\langle\hat{a}_{-\kappa\downarrow},\hat{a}_{-\kappa\downarrow}^\dagger\right\rangle\right\rangle$$
$$=-\frac{M}{\left(\omega-\epsilon_{-\kappa}\right)}-\left(\frac{M\Delta_{\mathrm{SC}}}{\left(\omega-\epsilon_{-\kappa}\right)}+\frac{M\Delta_{\mathrm{SC}}}{\left(\omega+\epsilon_{k-q}\right)}\right)\left\langle\left\langle\hat{a}_{\kappa\uparrow}^\dagger,\hat{a}_{-\kappa\downarrow}^\dagger\right\rangle\right\rangle. \tag{18}$$

Applying nesting condition $\epsilon_\kappa=-\epsilon_{\kappa\pm q}$, $\epsilon_{-\kappa}=\epsilon_{\kappa\mp q}$ and use approximation, $\epsilon_\kappa=\epsilon_{-\kappa}$; Equations (17) and (14) becomes:

$$\left(\omega+\epsilon_\kappa-\frac{M^2}{\left(\omega-\epsilon_\kappa\right)}-\frac{\Delta_{\mathrm{SC}}^2}{\left(\omega-\epsilon_k\right)}\right)\left\langle\left\langle\hat{a}_{\kappa\uparrow}^\dagger,\hat{a}_{-\kappa\downarrow}\right\rangle\right\rangle$$
$$=-\frac{\Delta_{\mathrm{SC}}}{\left(\omega-\epsilon_\kappa\right)}-\left(\frac{M\Delta_{\mathrm{SC}}}{\left(\omega-\epsilon_\kappa\right)}+\frac{M\Delta_{\mathrm{SC}}}{\left(\omega-\epsilon_\kappa\right)}\right)\left\langle\left\langle\hat{a}_{-k+q\downarrow},\hat{a}_{-\kappa\downarrow}^\dagger\right\rangle\right\rangle \tag{19}$$

and

$$\left(\left(\omega+\epsilon_k\right)-\frac{M^2}{\left(\omega-\epsilon_k\right)}-\frac{\Delta_{\mathrm{SC}}^2}{\left(\omega-\epsilon_\kappa\right)}\right)\left\langle\left\langle\hat{a}_{-\kappa\downarrow},\hat{a}_{-\kappa\downarrow}^\dagger\right\rangle\right\rangle$$
$$=-\frac{M}{\left(\omega-\epsilon_k\right)}-\left(\frac{M\Delta_{\mathrm{SC}}}{\left(\omega-\epsilon_k\right)}+\frac{M\Delta_{\mathrm{SC}}}{\left(\omega-\epsilon_k\right)}\right)\left\langle\left\langle\hat{a}_{\kappa\uparrow}^\dagger,\hat{a}_{-\kappa\downarrow}^\dagger\right\rangle\right\rangle. \tag{20}$$

Let $x=\omega+\epsilon_k$ and $y=\omega-\epsilon_k$.

Then Equations (19) and (20) respectively becomes:

$$\left[xy-M^2-\Delta_{\mathrm{SC}}^2\right]\left\langle\left\langle\hat{a}_{\kappa\uparrow}^{?},\hat{a}_{-\kappa\downarrow}\right\rangle\right\rangle=-\Delta_{\mathrm{SC}}-2M\Delta_{\mathrm{SC}}\left\langle\left\langle\hat{a}_{-k+q\uparrow},\hat{a}_{-\kappa\downarrow}\right\rangle\right\rangle \tag{21}$$

$$\left[xy-M^2-\Delta_{\mathrm{SC}}^2\right]\left\langle\left\langle\hat{a}_{-k+q\downarrow},\hat{a}_{-\kappa\downarrow}^{?}\right\rangle\right\rangle=-\Delta_{\mathrm{SC}}-2M\Delta_{\mathrm{SC}}\left\langle\left\langle\hat{a}_{\kappa\uparrow},\hat{a}_{-\kappa\downarrow}\right\rangle\right\rangle. \tag{22}$$

Finally we can express:

$$\left\langle\left\langle\hat{a}_{\kappa\uparrow}^\dagger,\hat{a}_{-\kappa\downarrow}^\dagger\right\rangle\right\rangle=\frac{-1/2\left(\Delta_{\mathrm{SC}}+M\right)}{\omega^2-\epsilon_\kappa^2-\left(\Delta_{\mathrm{SC}}+M\right)^2}+\frac{-1/2\left(\Delta_{\mathrm{SC}}-M\right)}{\omega^2-\epsilon_\kappa^2-\left(\Delta_{\mathrm{SC}}-M\right)^2}. \tag{23}$$

Using the expression $\omega\to i\omega_n,\Delta_j\left(k\right)=-\left(-1\right)^j M$, where $\Delta_j\left(k\right)$ is effective order parameter and the Matsubara's frequency, we can write Equation (23) as:

$$\left\langle\left\langle\hat{a}_{\kappa\uparrow}^\dagger,\hat{a}_{-\kappa\downarrow}^\dagger\right\rangle\right\rangle=\frac{1}{2}\sum_{j=1,2}\frac{\beta^2\Delta_j\left(k\right)}{\left(2n+1\right)^2\pi^2+\beta^2\left(\epsilon_\kappa^2+\Delta_j^2\left(k\right)\right)}. \tag{24}$$

To take into account the temperature dependence of order parameters, we shall write as:

$$\Delta_{\mathrm{SC}}=\frac{V}{\beta}\sum_{\kappa,n}\left\langle\left\langle\hat{a}_{\kappa\uparrow}^\dagger,\hat{a}_{-\kappa\downarrow}^\dagger\right\rangle\right\rangle \tag{25}$$

$$M=\frac{U}{\beta}\sum_{k}\left\langle\left\langle\hat{a}_{\kappa\uparrow}^\dagger,\hat{a}_{k-q\downarrow}\right\rangle\right\rangle \tag{26}$$

where $\beta = \frac{1}{KT}$.

Using Equation (24) into Equation (25), we obtain

$$\Delta_{\text{SC}} = \frac{V}{2} \sum_{\kappa,n,j=1,2} \frac{\beta \Delta_j(k)}{(2n+1)^2 \pi^2 + \beta^2 \left(\epsilon_\kappa^2 + \Delta_j^2(k)\right)}. \tag{27}$$

Let us use

$$\gamma = \beta\left(\epsilon_\kappa^2 + \Delta_j^2(k)\right)^{1/2} \tag{28}$$

and

$$\sum_{-\infty}^{\infty} \frac{1}{(2n+1)^2 \pi^2 + \gamma} = \frac{\tanh \gamma/2}{2\gamma}. \tag{29}$$

Plugging Equation (28) and Equation (29) in Equation (27), we get:

$$\Delta_{\text{SC}} = \frac{V}{4} \sum_{j=1,2} \frac{\Delta_j(k) \tanh \frac{\beta}{2}\left(\epsilon_\kappa^2 + \Delta_j^2(k)\right)^{1/2}}{\left(\epsilon_\kappa^2 + \Delta_j^2(k)\right)^{1/2}}. \tag{30}$$

For mathematical convenience, we replace the summation in (27) by integration. Thus

$$\sum_k \equiv \int_{-\hbar\omega_b}^{\hbar\omega_b} N(0)\, \mathrm{d}\epsilon_\kappa$$

where $N(0)$ is the density of states at the Fermi level.

The density of state $N(0) = N(2)_1 + N(0)_2$.

Assume $N(2)_1 = N(0)_2$ this implies that $N(0)_2 = N(0)/2$. For $j = 2$:

$$\Delta_{\text{SC}} = \alpha \int_0^{\hbar\omega_b} (\Delta_{\text{SC}} - M) \frac{\tanh \frac{\beta}{2}\left(\epsilon_\kappa^2 + (\Delta_{\text{SC}} - M)^2\right)^{1/2}}{\left(\epsilon_\kappa^2 + (\Delta_{\text{SC}} - M)^2\right)^{1/2}} \mathrm{d}\epsilon_\kappa \tag{31}$$

where $\alpha = N(0)_2 V$.

Finally we can write Equation (31) as:

$$\frac{1}{\alpha} = \int_0^{\hbar\omega_b} \left(1 - \frac{M}{\Delta_{\text{SC}}}\right) \frac{\tanh \frac{\beta}{2}\left(\epsilon_\kappa^2 + (\Delta_{\text{SC}} - M)^2\right)^{1/2}}{\left(\epsilon_\kappa^2 + (\Delta_{\text{SC}} - M)^2\right)^{1/2}} \mathrm{d}\epsilon_\kappa. \tag{32}$$

From (32), it clearly follows that the order parameters Δ_{SC} and M, for superconductivity and SDW are interdependent.

We now consider the equations of motion for SDW, we can write,

$$\omega \left\langle\left\langle \hat{a}_{\kappa\uparrow}^\dagger, \hat{a}_{k-q\downarrow} \right\rangle\right\rangle = \delta_{Kk'} + \left\langle\left\langle \left[\hat{a}_{\kappa\uparrow}^\dagger, H\right], \hat{a}_{k-q\downarrow} \right\rangle\right\rangle. \tag{33}$$

Doing a lot as we did in the above, we finally get:

$$(\omega + \epsilon_\kappa) \left\langle\left\langle \hat{a}_{\kappa\uparrow}^\dagger, \hat{a}_{k-q\downarrow} \right\rangle\right\rangle = -M \left\langle\left\langle \hat{a}_{\kappa-q\downarrow}^\dagger, \hat{a}_{k-q\downarrow} \right\rangle\right\rangle - \Delta_{\text{SC}} \left\langle\left\langle \hat{a}_{-k\downarrow}, \hat{a}_{k-q\downarrow} \right\rangle\right\rangle \tag{34}$$

$$(\omega + \epsilon_{\kappa-q}) \left\langle\left\langle \hat{a}_{\kappa-q\downarrow}^\dagger, \hat{a}_{k-q\downarrow} \right\rangle\right\rangle = 1 - M \left\langle\left\langle \hat{a}_{\kappa\uparrow}^\dagger, \hat{a}_{k-q\downarrow} \right\rangle\right\rangle + \Delta_{\text{SC}} \left\langle\left\langle \hat{a}_{-k+q\uparrow}, \hat{a}_{k-q\downarrow} \right\rangle\right\rangle \tag{35}$$

$$(\omega - \epsilon_{-\kappa+q}) \left\langle\left\langle \hat{a}_{-k+q\uparrow}, \hat{a}_{k-q\downarrow} \right\rangle\right\rangle = M \left\langle\left\langle \hat{a}_{-k\downarrow}, \hat{a}_{k-q\downarrow} \right\rangle\right\rangle + \Delta_{\text{SC}} \left\langle\left\langle \hat{a}_{\kappa-q\downarrow}^\dagger, \hat{a}_{k-q\downarrow} \right\rangle\right\rangle \tag{36}$$

and

$$(\omega-\epsilon_{-\kappa})\left\langle\left\langle\hat{a}_{-k\downarrow},\hat{a}_{k-q\downarrow}\right\rangle\right\rangle = M\left\langle\left\langle\hat{a}_{-k+q\uparrow},\hat{a}_{k-q\downarrow}\right\rangle\right\rangle - \Delta_{\mathrm{SC}}\left\langle\left\langle\hat{a}^{\dagger}_{\kappa\uparrow},\hat{a}_{k-q\downarrow}\right\rangle\right\rangle. \tag{37}$$

Doing a lot as we did in the previous, we finally get:

$$\left\langle\left\langle\hat{a}^{\dagger}_{\kappa\uparrow},\hat{a}_{k-q\downarrow}\right\rangle\right\rangle = \frac{1}{2}\sum_{j=1,2}\frac{(-1)^{j}\beta^{2}\Delta_{j}(k)}{(2n+1)^{2}\pi^{2}+\beta^{2}\left(\epsilon_{k}^{2}+\Delta_{j}^{2}(k)\right)}. \tag{38}$$

Using Equation (38) in to Equation (26), the SDW order Parameter M is given by:

$$M=-\frac{U}{2}\sum_{k,n,j=1}\frac{\beta\Delta_{j}(k)}{(2n+1)^{2}\pi^{2}+\beta^{2}\left(\epsilon_{\kappa}^{2}+\Delta_{j}^{2}(k)\right)} \tag{39}$$

or

$$M=\frac{-U}{4}\sum_{j=1}\frac{\Delta_{j}(k)\tanh\frac{\beta}{2}\left(\epsilon_{\kappa}^{2}+\Delta_{j}^{2}(k)\right)^{1/2}}{\left(\epsilon_{\kappa}^{2}+\Delta_{j}^{2}(k)\right)^{1/2}}. \tag{40}$$

So, finally we get:

$$M=-\alpha_{j}\Delta_{j}\int_{0}^{\hbar\omega_{b}}\frac{\tanh\frac{\beta}{2}\left(\epsilon_{\kappa}^{2}+\Delta_{j}^{2}(k)\right)^{1/2}}{\left(\epsilon_{\kappa}^{2}+\Delta_{j}^{2}(k)\right)^{1/2}}\mathrm{d}\epsilon_{\kappa}. \tag{41}$$

From (41), it is again evident that the order parameters Δ_{SC} and M, for superconductivity and SDW are interdependent, as was the case from (32).

It is, therefore, possible that in some temperature interval, SDW and superconductivity can co-exist, although one phase has a tendency to suppress the critical temperature and the order parameter of the other phase.

2.2. Dependence of the Magnetic Order Parameter on the Transition Temperature for Spin Density Wave and Superconductivity

To study Equation (32), we consider the case, when $T\to 0\ \mathrm{K}, \beta\to\infty$.

We can then replace

$$\tanh\frac{\beta}{2}\left(\epsilon_{\kappa}^{2}+(\Delta_{\mathrm{SC}}-M)^{2}\right)^{1/2}\to 1.$$

In (32) and get,

$$\frac{1}{\alpha}=\int_{0}^{\hbar\omega_{b}}\left(1-\frac{M}{\Delta_{\mathrm{SC}}}\right)\frac{1}{\left(\epsilon_{\kappa}^{2}+(\Delta_{\mathrm{SC}}-M)^{2}\right)^{1/2}}\mathrm{d}\epsilon_{\kappa}.$$

Using the integral relation,

$$\int\frac{y}{\sqrt{y^{2}+x^{2}}}\mathrm{d}x = y\sin^{-1}(x/y)$$

$$\frac{1}{\alpha}=\left(1-\frac{M}{\Delta_{\mathrm{SC}}}\right)\sin^{-1}\frac{(\hbar\omega_{b})}{(\Delta_{\mathrm{SC}}-M)} \tag{42}$$

the above equation reduces to,

$$\Delta_{\mathrm{SC}}-M=2\hbar\omega_{b}\exp\left(-\frac{1}{\alpha\left(1-\frac{M}{\Delta_{\mathrm{SC}}}\right)}\right) \tag{43}$$

from the BCS theory, the order parameter Δ_{SC}, at $T = 0$ for a given superconductor with transition temperature T_C is given by

$$2\Delta_{\text{SC}}(0) = 3.53 k_B T_c \tag{44}$$

using this result in (43), we obtain

$$M = 1.75 k_B T_c - 2\hbar\omega_b \exp\left(-\frac{1}{\alpha\left(1-\frac{M}{1.75 k_B T_c}\right)}\right). \tag{45}$$

To solve (45) numerically we use Debay temperature and the interband BCS coupling constant.
To estimate α, I consider the case $T \to T_c$ which implies, $\Delta_{\text{SC}} \to 0$.
From (32), we then have

$$\frac{1}{\alpha} = \int_0^{\hbar\omega_b} \frac{\tanh\frac{\beta}{2}\left(\epsilon_\kappa^2 + (\Delta_{\text{SC}} - M)^2\right)^{1/2}}{\left(\epsilon_\kappa^2 + (\Delta_{\text{SC}} - M)^2\right)^{1/2}} \mathrm{d}\epsilon_\kappa - \int_0^{\hbar\omega_b} \frac{M}{\Delta_{\text{SC}}} \frac{\tanh\frac{\beta}{2}\left(\epsilon_\kappa^2 + (\Delta_{\text{SC}} - M)^2\right)^{1/2}}{\left(\epsilon_\kappa^2 + (\Delta_{\text{SC}} - M)^2\right)^{1/2}} \mathrm{d}\epsilon_\kappa$$

$$\frac{1}{\alpha} = I_1 - I_2 \tag{46}$$

$$\frac{1}{\alpha} = \int_0^{\hbar\omega_b} \frac{\tanh\frac{\beta}{2}\left(\epsilon_\kappa^2 + (\Delta_{\text{SC}} - M)^2\right)^{1/2}}{\left(\epsilon_\kappa^2 + (\Delta_{\text{SC}} - M)^2\right)^{1/2}} \mathrm{d}\epsilon_\kappa - \lim_{\Delta_{\text{SC}}\to 0} \int_0^{\hbar\omega_b} \frac{M}{\Delta_{\text{SC}}} \frac{\tanh\frac{\beta}{2}\left(\epsilon_\kappa^2 + (\Delta_{\text{SC}} - M)^2\right)^{1/2}}{\left(\epsilon_\kappa^2 + (\Delta_{\text{SC}} - M)^2\right)^{1/2}} \mathrm{d}\epsilon_\kappa.$$

Putting $\tau^2 = \beta\sqrt{\epsilon_\kappa^2 + M^2}$ and for $\Delta_{\text{SC}} = 0$ we can write

$$I_1 = \int_0^{\hbar\omega_b} \frac{\tanh\frac{\beta}{2}\left(\epsilon_\kappa^2 + M^2\right)^{1/2}}{\left(\epsilon_\kappa^2 + M^2\right)^{1/2}} \mathrm{d}\epsilon_\kappa = \int_0^{\hbar\omega_b} \frac{2}{2\tau}\beta \tanh\frac{\tau}{2} \mathrm{d}\epsilon_\kappa. \tag{47}$$

Using Laplacian's transformation with Matsuber relation result we can write,

$$\int_0^{\hbar\omega_b} \frac{\tanh\frac{\beta}{2}\left(\epsilon_\kappa^2 + M^2\right)^{1/2}}{\left(\epsilon_\kappa^2 + M^2\right)^{1/2}} \mathrm{d}\epsilon_\kappa = \int_0^{\hbar\omega_b} \frac{\tanh\frac{\beta\epsilon_\kappa}{2}}{\epsilon_\kappa} \mathrm{d}\epsilon_\kappa - \int_0^{\hbar\omega_b} \frac{4}{\beta} \sum_{n=0}^{\infty} \frac{M^2}{a^4\left(1+x^2\right)^2}$$

where $x^2 = \frac{\epsilon_\kappa^2}{a^2}$ and $a = (2n+1)\frac{\pi}{\beta}$ and using integrating by part,

$$\int_0^{\hbar\omega_b} \frac{\tanh\frac{\beta}{2}\left(\epsilon_\kappa^2 + M^2\right)^{1/2}}{\left(\epsilon_\kappa^2 + M^2\right)^{1/2}} \mathrm{d}\epsilon_\kappa = (\ln x)(\tanh x)\Big|_0^x - \int_0^x \frac{\ln x}{\cosh^2 x} \mathrm{d}x - \int_0^{\hbar\omega_b} \frac{4}{\beta} \sum_{n=0}^{\infty} \frac{M^2}{a^4\left(1+x^2\right)^2}$$

$$\int_0^{\hbar\omega_b} \frac{\tanh\frac{\beta}{2}\left(\epsilon_\kappa^2 + M^2\right)^{1/2}}{\left(\epsilon_\kappa^2 + M^2\right)^{1/2}} \mathrm{d}\epsilon_\kappa = \ln\frac{\beta\hbar\omega_b}{2} - \ln\left(\frac{\pi}{4\gamma}\right) - M^2\left(\frac{1}{\pi k_\beta T_{SC}}\right)^2 1.052. \tag{48}$$

Using the fact that, for low temperature, $\tanh\left(\frac{\hbar\omega_b}{2k_B T}\right) \to 1$, where γ is the Euler constant having the value $\gamma = 1.78$ (Hsian) [15] and the last equation can be neglected since M^2 is very small.

We can write (48) as,

$$I_1 = \ln\left(1.14\frac{\hbar\omega_b}{k_B T_{sc}}\right). \quad (49)$$

Using L'Hospital's rule, it is easy to show that

$$I_2 = -\int_0^{\hbar\omega_b}\left(M^2\beta\right)\frac{\operatorname{sech}^2\left(\frac{\beta\sqrt{\epsilon_\kappa^2+M^2}}{2}\right)}{2\left(\epsilon_\kappa^2+M^2\right)}\mathrm{d}\epsilon_\kappa$$

which can be neglected since M_{SDW}^2 is very small.

Substituting (49) in (46), we then obtain

$$\frac{1}{\alpha} = \ln\left(1.14\frac{\hbar\omega_b}{k_B T_C}\right).$$

This implies,

$$T_C = \frac{1.14\hbar\omega_b}{k_B}\exp\left(-\frac{1}{\alpha}\right), \quad (50)$$

which can be used to estimate $\exp\left(-\frac{1}{\alpha}\right)$ for $Ba_{1-x}K_xFe_2As_2$, using the experimental value T_C and cut-off energy.

To study how *M* depends on the magnetic transition temperature T_{SDW}, we consider (41).

$$M = -\alpha_j\Delta_j\int_0^{\hbar\omega_b}\frac{\tanh\frac{\beta}{2}\left(\epsilon_\kappa^2+\Delta_j^2(k)\right)^{1/2}}{\left(\epsilon_\kappa^2+\Delta_j^2(k)\right)^{1/2}}\mathrm{d}\epsilon_\kappa \quad (51)$$

proceeding as before, it is easy to show that,

$$M = -\alpha_j\Delta_j\left(\ln\left(1.14\frac{\hbar\omega_b}{k_B T_{SDW}}\right)-\Delta_j^2\left(\frac{1}{\pi k_\beta T_{SDW}}\right)^2 1.052\right).$$

Neglecting Δ_j^2

$$M = -\left(\alpha_j\Delta_j\right)\ln\left(1.14\frac{\hbar\omega_b}{k_B T_{SDW}}\right).$$

This gives;

$$\therefore T_{SDW} = \left(\frac{1.14\hbar\omega_b}{k_B}\right)\exp\left(\frac{M}{\alpha_j\Delta_j}\right) \quad (52)$$

we can use (52) to draw the phase diagram for *M* and T_{SDW}.

2.3. Pairing of Spin Density Wave (SDW) and Triplet Superconductivity

In this section we want to drive an expressions for the order parameters of SDW, *M*, and triplet superconductivity, Δ_{SC}, as a function of both of them and temperature, and to compare the variation of each with temperature. Still we can use the Hamiltonian given by Equation (1), but in this case the superconducting order parameter depends on spin alignment [16] and they can be expressed as;

$$H = \sum_{p\sigma}\epsilon_p\hat{a}_{p\sigma}^{\dagger}\hat{a}_{p\sigma} + M\sum_p\left(\hat{a}_{p+q\uparrow}^{\dagger}\hat{a}_{-p\downarrow}+\hat{a}_{-p\downarrow}^{\dagger}\hat{a}_{p+q\uparrow}\right)+\Delta_{SC}\sum_p\left(\hat{a}_{p\uparrow}^{\dagger}\hat{a}_{-p\downarrow}^{\dagger}+\hat{a}_{-p\downarrow}\hat{a}_{p\uparrow}\right) \quad (53)$$

where the superconducting order parameter is given by:

$$\Delta = \sum_{P} \left\langle \hat{a}^{\dagger}_{k\sigma}, \hat{a}^{\dagger}_{-k\sigma} \right\rangle. \tag{54}$$

We now consider the equation of motion:

$$\omega \left\langle\left\langle \hat{a}^{\dagger}_{\kappa\sigma}, \hat{a}^{\dagger}_{-\kappa\sigma} \right\rangle\right\rangle = \left\langle\left\langle \left[\hat{a}^{\dagger}_{\kappa\sigma}, H \right], \hat{a}^{\dagger}_{-\kappa\sigma} \right\rangle\right\rangle. \tag{55}$$

Doing a lot as we did in the above for the commutation and using the assumption $\delta_{\sigma,\downarrow} = 1, \delta_{\sigma,\uparrow} = 0$ we finally get:

$$(\omega + \epsilon_{\kappa}) \left\langle\left\langle \hat{a}^{\dagger}_{\kappa\downarrow}, \hat{a}^{\dagger}_{-\kappa\downarrow} \right\rangle\right\rangle = -M \left\langle\left\langle \hat{a}^{\dagger}_{\kappa+q\uparrow}, \hat{a}^{\dagger}_{-\kappa\downarrow} \right\rangle\right\rangle - \Delta_{k\downarrow} \left\langle\left\langle \hat{a}_{-k\downarrow}, \hat{a}^{\dagger}_{-\kappa\downarrow} \right\rangle\right\rangle. \tag{56}$$

The nesting property of the Fermi surface that expected for low dimensional band structure and attributed to the SDW ordering gives as an expression $\Delta_{-k} = -\Delta_{k}$.

Finally:

$$(\omega + \epsilon_{\kappa}) \left\langle\left\langle \hat{a}^{\dagger}_{\kappa\downarrow}, \hat{a}^{\dagger}_{-\kappa\downarrow} \right\rangle\right\rangle = -\Delta_{k\downarrow} \left\langle\left\langle \hat{a}_{-k\downarrow}, \hat{a}^{\dagger}_{-\kappa\downarrow} \right\rangle\right\rangle. \tag{57}$$

Since we are dealing with only the triplet pair; we can ignore the singlet correlation.

The equation of motion for correlation in RHS of (57) is written as:

$$(\omega - \epsilon_{-\kappa}) \left\langle\left\langle \hat{a}_{-k\downarrow}, \hat{a}^{\dagger}_{-k\downarrow} \right\rangle\right\rangle = 1 + M \left\langle\left\langle \hat{a}_{-k+q\uparrow}, \hat{a}^{\dagger}_{-\kappa\downarrow} \right\rangle\right\rangle - \Delta_{k\downarrow} \left\langle\left\langle \hat{a}^{\dagger}_{\kappa\downarrow}, \hat{a}^{\dagger}_{-\kappa\downarrow} \right\rangle\right\rangle \tag{58}$$

and

$$(\omega - \epsilon_{-\kappa+q}) \left\langle\left\langle \hat{a}_{-k+q\uparrow}, \hat{a}^{\dagger}_{-k\downarrow} \right\rangle\right\rangle = M \left\langle\left\langle \hat{a}_{-k\downarrow}, \hat{a}^{\dagger}_{-\kappa\downarrow} \right\rangle\right\rangle \tag{59}$$

which can be rewritten, after solving the commutation relation and removing the singlet pair.

From Equations (58) and (59), we will get;

$$(\omega - \epsilon_{-\kappa}) \left\langle\left\langle \hat{a}_{-k\downarrow}, \hat{a}^{\dagger}_{-k\downarrow} \right\rangle\right\rangle = 1 + \frac{M^2}{(\omega - \epsilon_{\kappa+q})} \left\langle\left\langle \hat{a}_{-k\downarrow}, \hat{a}^{\dagger}_{-k\downarrow} \right\rangle\right\rangle - \Delta_{k\downarrow} \left\langle\left\langle \hat{a}^{\dagger}_{\kappa\downarrow}, \hat{a}^{\dagger}_{-\kappa\downarrow} \right\rangle\right\rangle. \tag{60}$$

With help of Equation (60) and Equation (57):

$$\frac{XYR - XM^2 - R\Delta^2_{K\downarrow}}{YR - M^2} \left\langle\left\langle \hat{a}^{\dagger}_{\kappa\downarrow}, \hat{a}^{\dagger}_{-\kappa\downarrow} \right\rangle\right\rangle = \frac{-\Delta_{K\downarrow}}{YR - M^2} \tag{61}$$

which in turn can be written as:

$$\left\langle\left\langle \hat{a}^{\dagger}_{\kappa\downarrow}, \hat{a}^{\dagger}_{-\kappa\downarrow} \right\rangle\right\rangle = \frac{-\Delta_{K\downarrow} R}{XYR - XM^2 - R\Delta^2_{K\downarrow}}. \tag{62}$$

Applying nesting condition $\epsilon_{\kappa} = -\epsilon_{\kappa\pm q}$, $\epsilon_{-\kappa} = \epsilon_{\kappa\mp q}$ and use approximation, $\epsilon_{\kappa} = \epsilon_{-\kappa}$; Equation (62) becomes:

$$\left\langle\left\langle \hat{a}^{\dagger}_{\kappa\downarrow}, \hat{a}^{\dagger}_{-\kappa\downarrow} \right\rangle\right\rangle = \frac{-\Delta_{K\downarrow}}{XY - M^2 - \Delta^2_{K\downarrow}} \tag{63}$$

Using the expression $\omega \to i\omega_n$, Equation (29) and Matsubara's frequency, we can write Equation (63) as:

$$\Delta_{k'\downarrow} = V \sum_{k} \frac{\Delta_{k\downarrow} \tanh \dfrac{\left(\sqrt{\epsilon^2_{\kappa} + M^2 + \Delta^2_{k\downarrow}}\right)}{2k_B T}}{2\sqrt{\epsilon^2_{\kappa} + M^2 + \Delta^2_{k\downarrow}}} \tag{64}$$

where

$$\Delta_{k'\downarrow} = \frac{V}{\beta}\sum_{k,n}\left\langle\left\langle \hat{a}^{\dagger}_{\kappa\downarrow}, \hat{a}^{\dagger}_{-\kappa\downarrow}\right\rangle\right\rangle$$

$$\Delta_{k'\downarrow} = \frac{V}{\beta}\sum_{k,n}\frac{\Delta_{K\downarrow}}{\omega_n^2 + E_k^2}$$

and $E_k^2 = \epsilon_\kappa^2 + M^2 + \Delta_\downarrow^2$.

By taking an approximation over the superconducting order parameter, such that it is independent of wave vector, finally we get:

$$1 = V\sum_k \frac{\tanh\dfrac{\left(\sqrt{\epsilon_\kappa^2 + M^2 + \Delta_\downarrow^2}\right)}{2k_B T}}{2\sqrt{\epsilon_\kappa^2 + M^2 + \Delta_\downarrow^2}}. \tag{65}$$

We now consider the equations of motion for SDW, we can write,

$$\omega\left\langle\left\langle \hat{a}^{\dagger}_{\kappa\uparrow}, \hat{a}_{k-q\downarrow}\right\rangle\right\rangle = \left\langle\left\langle \left[\hat{a}^{\dagger}_{\kappa\sigma}, H\right], \hat{a}^{\dagger}_{-\kappa\sigma}\right\rangle\right\rangle. \tag{66}$$

Doing a lot as we did in the above, we finally get:

$$\left\langle\left\langle \hat{a}^{\dagger}_{\kappa\uparrow}, \hat{a}_{k-q\downarrow}\right\rangle\right\rangle = \frac{-M}{XZR - \Delta_{k-q\downarrow}^2 X - M^2 R}. \tag{67}$$

So,

$$1 = U\sum_k \frac{\tanh\dfrac{\left(\sqrt{\epsilon^2 + \Delta_\downarrow^2 + M^2}\right)}{2k_B T}}{2\sqrt{\epsilon^2 + \Delta_\downarrow^2 + M^2}}. \tag{68}$$

3. Results

Starting with a model Hamiltonian for the system and using Green's function formalism, we obtained expressions for superconducting transition temperature (T_C), magnetic order parameter (M) and spin density wave transition temperature (T_{SDW}). Based on these result we found two very vital equations ((45) and (52)). Moreover, we scrutinized the effect of magnetic order parameter (M) on superconducting transition temperature (T_C) and spin density wave transition temperature (T_{SDW}) in $Ba_{1-x}K_xFe_2As_2$ by using the relevant parameters. For this purpose, we have used (45) which have been numerically solved using the relevant parameters to plot the phase diagram for magnetic order parameter (M) versus superconducting transition temperature (T_C). In the same figure, we have also plotted the phase diagram of magnetic ordering (M) versus spin density wave transition temperature (T_{SDW}), using (52). From the graph we observe T_C decreases with increase in M, whereas T_{SDW} increases with increase in M. The phase diagrams of M versus T_C and M versus T_{SDW}, were merged to obtain the region where both spin density wave and superconductivity co-exist. The regions of intersection of the two merged graphs showed in **Figure 1** indicate co-existence of spin density wave and superconductivity for $Ba_{1-x}K_xFe_2As_2$.

4. Conclusion

Using a model Hamiltonian consisting of spin density wave and superconducting part and applying Green's function formalism we have got an expression which shows the relation of the two order parameters and their variation with temperature. From **Figure 1** we observe that T_C decreases with increase in M, whereas T_{SDW} increases with increase in M. The spin density wave and superconducting phases, therefore, resist each other. However, the present work shows that there is a small region of temperature, where both the phases may be in existence together, which is indicated by (SC + SDW) in the figure. In the absence of spin density wave the expression for both singlet and triplet cases reduces to the well known BCS result. My study explicitly shows that

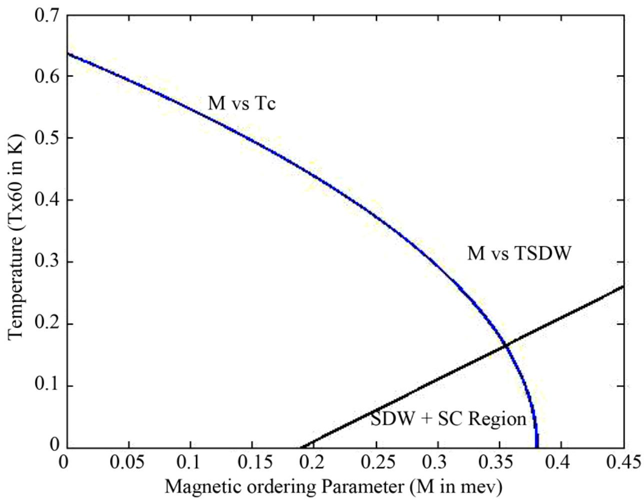

Figure 1. Co-existence of spin density wave (SDW) and superconductivity in $Ba_{1-x}K_xFe_2As_2$.

spin density wave and superconductivity truly coexist in $Ba_{1-x}K_xFe_2As_2$ ($0.2 \le x < 0.4$) in some range of magnetic order.

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