Theoretical Study of the Interplay of Superconductivity and Magnetism in FeAs Based Superconductors

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Abstract

The interaction of superconductivity and magnetism is studied in iron based superconductor using the Hamiltonian consisting of the itinerant electrons, localized electrons moment, and s-f interaction. Using Greens function technique and equation of motion method, we have obtained an expressions for superconducting order parameters $\left(\Delta(T), \Delta(0) \right)$ and critical temperature T_C, which reduce to BCS result in the absence of magnetic interactions. The result of the calculations shows that superconductivity can coexist with magnetism in iron based superconductor below the critical temperature.

1. Introduction

The discovery of high T_C iron based superconductor in 2008 [1] boosts multidirectional investigation from experimental as well as theoretical views. Nowadays, understanding the mechanism of superconductivity in such system is one of the challenging research areas. According to reviews on iron based superconductors [2] [3], magnetic interactions are important for understanding the mechanism of superconductivity. Experimental observation and theoretical prediction show that knowing the interplay of superconductivity and magnetism may suggest the possible mechanism of superconductivity.

The interplay of superconductivity and magnetism has been studied in iron based superconductors theoretically and experimentally [4] [5]. Superconductivity could be obtained applying either external pressure or dop-

ing. In most iron based superconductors, both electron and hole doping on parent compounds cause superconductivity. Upon doping, for example, potassium doping magnetism gradually disappears with a lowering of the spin density wave transition temperature [6]. In systems like $CeFeAsO_{1-x}F_x$, magnetism is suppressed by doping before the appearance of superconductivity [7]. Generally substitution of element in the 122 parent compounds may lead to suppression of spin density wave and eventual appearance of superconductivity [4] [8]. Some compounds show a coexistence of magnetism and superconductivity [9]-[11]

In this work, we are trying to predict the interplay of superconductivity and magnetism on iron based superconductors which can help in explaining experimental observations.

2. The Model Hamiltonian

Our model Hamiltonian is composed of

$$H = H_P + H_l + H_{el}, \qquad (1)$$

where the first term, $H_p = \sum_{k,\sigma} \varepsilon(k) \hat{a}_{k\sigma}^\dagger \hat{a}_{k\sigma} - \sum_{kk'} V_{kk'} \hat{a}_{k\uparrow}^\dagger \hat{a}_{-k\downarrow}^\dagger \hat{a}_{-k'\downarrow} \hat{a}_{k'\uparrow}$.

In the above pairing Hamiltonian the term

$$\sum_{k,\sigma} \varepsilon(k) \hat{a}_{k\sigma}^\dagger \hat{a}_{k\sigma},$$

describes the Hamiltonian of total energy of the itinerant electrons in one electron band approximation [12]. Here the operators $\hat{a}_{k\sigma}^\dagger (\hat{a}_{k\sigma})$ creates (annihilates) an electron with the wave vector k and the spin projection on z-axis $\sigma = \uparrow$ or $\downarrow$; $V_{kk'}$ is the BCS pair potential. The second term $\left(H_l = \sum_{i,j} JS_i \cdot S_j \right)$ describes the predominant interaction between the local moment by Heisenberg like model, and we considered only the nearest neighbor interaction. Here J is the nearest neighbor exchange that bridge by the As ions and it could be anti ferromagnetic in nature. The third term $\left(H_{el} = -g \sum_i \sigma_i \cdot S_i \right)$ describes the interaction between the spin σ_i of the itinerant electrons and the five 3d spin S_i local moment located at site i, where g is the corresponding exchange constant.

To get an effective interaction we change the momentum term in to boson operator. Diagonalizing the Hamiltonian (H_l) using Bogoliubov transformation, the canonical form of the Hamiltonian in terms of spin waves,

$$H_l = E_O + \sum_k \omega_k b_k^\dagger b_k \qquad (2)$$

We obtained the itinerant electrons and localized electrons moment using relations in spin operators like,

$$S_i^\sigma = \hat{a}_{i\sigma}^\dagger \hat{a}_{i-\sigma}, \quad \frac{1}{\hbar}\sigma_i^\dagger = \hat{a}_{i\downarrow}^\dagger \hat{a}_{i\uparrow}, \quad \frac{1}{\hbar}\sigma_i^z = \frac{1}{2}\sum_\sigma z_\sigma n_{i\sigma}; \quad \left(z_\uparrow = +1; z_\downarrow = -1 \right).$$

The electrons in the valence band which are interacting with an anti ferromagnetically ordered, localized spin system can be described by

$$H_{el} = -\frac{1}{2} g \left\langle S^z \right\rangle \sum_{k,\sigma} \hat{a}_{k\sigma}^\dagger \hat{a}_{k\sigma} \qquad (3)$$

We get an effective Hamiltonian

$$H_{eff} = \sum_{k,\sigma} \varepsilon(k) \hat{a}_{k\sigma}^\dagger \hat{a}_{k\sigma} - \sum_{kk'} V_{kk'} \hat{a}_{k\uparrow}^\dagger \hat{a}_{-k\downarrow}^\dagger \hat{a}_{-k'\downarrow} \hat{a}_{k'\uparrow} + E_O + \sum_k \omega_k \hat{b}_k^\dagger \hat{b}_k - \frac{1}{2} g \hbar \left\langle S^z \right\rangle \sum_{k\sigma} \hat{a}_{k\sigma}^\dagger \hat{a}_{k\sigma} \qquad (4)$$

In order to calculate the superconducting parameter, we first need to obtain equation of motion. In this work we used Greens function equation of motion method. Applying elementary commutation relation we found two equations:

$$(\omega - \varepsilon) \left\langle\!\left\langle a_{-k\downarrow}^\dagger, a_{k'\uparrow}^\dagger \right\rangle\!\right\rangle \gg = -\Delta \left\langle\!\left\langle a_{k'\uparrow}, a_{k'\uparrow}^\dagger \right\rangle\!\right\rangle \qquad (5a)$$

$$(\omega + \varepsilon) \left\langle\!\left\langle a_{k'\uparrow}, a_{k'\uparrow}^\dagger \right\rangle\!\right\rangle = 1 - \Delta \left\langle\!\left\langle a_{-k\downarrow}^\dagger, a_{k'\uparrow}^\dagger \right\rangle\!\right\rangle \qquad (5b)$$

From these we get,

$$\langle\langle a^\dagger_{-k\downarrow}, a^\dagger_{k'\uparrow}\rangle\rangle = \frac{-\Delta}{\omega^2 - \varepsilon^2 - \Delta^2} \tag{6}$$

where $\varepsilon = \varepsilon_k - 1/2\left(g\hbar\langle S^z\rangle\right)$ and $\langle\langle...\rangle\rangle$ is the abbreviated notation for the Green functions.

The superconducting order parameter can be expressed as

$$\Delta = \sum_{k,n} \frac{V_{kk'}}{\beta}\langle\langle a^\dagger_{-k\downarrow}, a^\dagger_{k'\uparrow}\rangle\rangle \tag{7}$$

The sum may be changed to integral by introducing the density of state $N(\varepsilon)$ and the above equation becomes

$$1 = \frac{1}{\beta}\sum \int d\varepsilon_o N(\varepsilon) V_{kk'}\left[\frac{-1}{\omega^2 - \varepsilon^2 - \Delta^2}\right] \tag{8}$$

Attractive interaction is effective for the region $-\hbar\omega_O < \varepsilon < \hbar\omega_O$ and assuming the density of states does not vary over this integral, then the expression becomes,

$$\frac{1}{\lambda} = \int_0^{\hbar\omega_0} \frac{2}{\beta}\sum_0^\infty \frac{-1}{\omega^2 - \varepsilon^2 - \Delta^2} \tag{9}$$

Applying Laplaces transform with replacement of ω by Matsubara frequency $\omega_n = (2n+1)\pi/\beta$, and using the approximation,

$$\frac{1}{\omega_n^2 + \varepsilon^2 + \Delta^2} \approx \frac{1}{\omega_n^2 + \varepsilon^2} - \frac{\Delta^2}{\left(\omega_n^2 + \varepsilon^2\right)^2}$$

The equation becomes

$$\frac{1}{\lambda} = \sum_0^{\hbar\omega_0} d\varepsilon \frac{\tanh(\beta/2)\varepsilon}{\varepsilon} - 4\Delta^2 \sum_{n=0}^\infty \left(\frac{\beta}{\pi(2n+1)^2}\right)^3 \int_0^\infty \frac{1}{\left(1+x^2\right)^2} dx \tag{10}$$

For low temperature the first integral becomes

$$I_1 = \ln\frac{1.13}{K_B T}\left(\hbar\omega_0 - \frac{1}{2}g\hbar\langle S^z\rangle\right)$$

The second integral becomes

$$I_2 = 1.05\left(\frac{\Delta}{\pi K_B T}\right)^2$$

Hence,

$$\frac{1}{\lambda} = \ln\frac{1.13}{K_B T}\left(\hbar\omega_0 - \frac{1}{2}g\hbar\langle S^z\rangle\right) - 1.05\left(\frac{\Delta}{\pi k_B T}\right)^2$$

This expression can be rewritten as

$$K_B T = 1.13\left(\hbar\omega_0 - \frac{1}{2}g\hbar\langle S^z\rangle\right)e^{-\left[\frac{1}{\lambda} + \left(\frac{\Delta}{\pi k_B T}\right)^2\right]} \tag{11}$$

3. Result

From this equation we can get the following important relations.

1) Superconducting order parameter as a function of temperature

$$\Delta(T) = \pi k_B T \sqrt{\left(\ln \frac{1.13\left(\hbar\omega_0 - 1/2\left(g\hbar\langle S^z\rangle\right)\right)}{k_B T}\right) - \frac{1}{\lambda}} \tag{12}$$

This quantity (Δ) is zero at critical temperature T_C. Substituting $\Delta = 0$, we get

$$K_B T = 1.13\left(\hbar\omega_0 - \frac{1}{2}g\hbar\langle S^z\rangle\right)e^{-\frac{1}{\lambda}} \tag{13}$$

2) using $\ln(1-x) = x - x^2/2 + \cdots$, $\ln T/T_C \approx -(1 - T/T_C)$ we get the well known equation

$$\Delta(T) = 3.06 k_B T_C \left(1 - \frac{1}{T_C}\right)^2$$

Or

$$\ln(T_C/T) = \left(\frac{\Delta}{\pi k_B T}\right)^2 \tag{14}$$

3) Equation (9) can be written as

$$\frac{1}{\lambda} = \sum_0^{\hbar\omega_0} d\varepsilon \frac{\tanh \beta / 2\sqrt{\varepsilon^2 + \Delta^2}}{\sqrt{\varepsilon^2 + \Delta^2}} \tag{15}$$

As $T \to 0$, and $\beta \to 0$, gives

$$\frac{1}{\lambda} = \int \frac{d\varepsilon}{\sqrt{\varepsilon^2 + \Delta^2}} \tag{16}$$

Applying standard integrals and approximation for $x \ll 1$, and $(1+x)^n \approx 1 + nx$, we get

$$\Delta(T \to 0) = \sqrt{4(\hbar\omega_0)^2 \exp(-1/\lambda) - \left(\frac{1}{2}g\hbar\langle S^z\rangle\right)^2} \tag{17}$$

4. Conclusions

Equation (13) is clearly in agreement with the fact that as the net magnetization increases, the induction of superconductivity decreases. In addition to this, in the absence of magnetic term, Equation (13) reduces to the well known BCS expression.

The results clearly show that superconductivity can coexist with magnetism in iron based superconductor below the critical temperature. Experimental findings show the coexistence of superconductivity and magnetism in some range of doping in some compounds [9]-[11]. Our theoretical predictions are in broad agreement with experimental findings [9]-[11], and the result may help in explaining experimental observations.

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