Role of electronic polarization of As-ions in iron Pnictide superconductors

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ABSTRACT *The role of screening term due to electronic polarization of As-ions, V_p in iron-pnictide superconductors has been studied using Green function technique for $LaFeAsO_{1-x}F_x$ compound. Expression for superconducting order parameter and transition temperature Tc has been obtained for this compound. The expression clearly indicates the dependence of superconducting order parameter and transition temperature on V_p .The result shows that transition temperature Tc increases with increasing V_p . This shows that electronic polarization of As- ions V_p helps to increase transition temperature Tc in this Compound.*

***Keywords**: electronic polarization, iron-pnictide, superconducting order parameter, transition temperature .*

INTRODUCTION

In 2008 the discovery of iron pnictides superconductor having Tc up to 55 K (3,1,15) has been done. This is different family from cuprates superconductor, where large Tc's can be achieved. This has provided another system where phenomenon of high critical temperature (Tc) of superconductivity can be explored to obtain new insight. Now the interest generated is not only because of the high transition temperature (Tc) but also due to the presence of iron atoms with arsenic atom in these compounds. Fe based superconductor have layered structure in alternate FeAs and LnO layers with superconductivity proposed to be in FeAs layers (4,5,6,7,15) . Each iron (Fe) atom is surrounded by four arsenic (As) atoms in a distorted tetrahedral geometry. Fe atoms form a square lattice, while arsenic (As) atoms located at the middle of each square are displaced above and below the Fe plane(2,15). On other hand, external pressure at optimized doping could also result in effective enhancement of Tc (3,8,9,10,11). The pairing mechanism in Fe based superconductor of these compound inspiration for spin fluctuation (SF)(14). The repulsive interaction is effective only if the coupling constant for scattering of pair from the hole to the electron band(14). That is much larger than the intra-band (repulsive) couplings, and orders to increase Tc in multiband system (14,12) the intra-band pairing should contribute positively to Tc (14,13). The electron phonon interaction (EPI) is due to electronic polarization (14) and electronic polarization (EPI_{pol}) is induced on vibration of As-ions and dependent on distance between Fe and As ions. Electronic polarization (EPI_{pol}) is also effected thermodynamic potential (G) as a function of the pressure and magnetic order parameter and strain. Electron phonon interaction (EPI) due to Electronic polarization of As ions play in the most important role to understand the mechanism behind these Fe-As based superconductors. Hence in the present work, the role of electronic polarization of As- ions (V_p) on the superconducting order parameter and transition temperature in iron-pnictide superconductors will be explore using Green function technique.

Mathematical formulation

In this present work double time retarded Green's function technique have been used as Mathematical tool for investigation of superconducting order parameter Δ and transition temperate Tc .
An appropriate model Hamiltonian for our system can be describe as

$$H = H_{0e} + H_{sup} + H_{pol} \tag{1}$$

Where,
H_{oe} is kinetic Energy of the conduction electron
H_{sup} is superconducting part describe BCS type
H_{Pol} is Part of Polarization of As- ions
Equation (1) can be written as

$$H = \sum_{k\sigma} \epsilon_k C_{k\sigma}^{+} C_{k\sigma} - \sum_{kk\prime\sigma} V_s C_{k\sigma}^{+} C_{-k\prime\sigma\prime}^{+} C_{-k\prime\sigma\prime} C_{k\prime\sigma} - \sum_{k\sigma} \frac{V_P}{2} C_{k\sigma}^{+} C_{k\sigma} + \sum_{kk'\sigma} U C_{k\sigma}^{+} C_{-k\sigma'}^{+} C_{-k'\sigma'} C_{k'\sigma} \quad (2)$$

Where $C_{k\sigma,}^{+}$ and $C_{k\sigma}$denoted the fermions creation and annihilation operator respectively, where k is Wave vector and σ is spin index for fermions .

In equation (2) The first term represent the kinetic energy of conduction Electron .The second term represent the formation of cooper pair, V_s superconductive attractive potential , U screened Hubbard repulsion , The third term represent in the term of V_p is screen term due to electronic polarization of As – ions .

In our present analysis we use a Green function, define as

$$G_{qq}^{\uparrow\uparrow} = \ll C_{q\uparrow} C_{q\uparrow}^{+} \gg \quad (3)$$

And writing equation of motion as

$$\omega G_{qq}^{\uparrow\uparrow} = \frac{1}{2\pi} + \langle\langle [C_{q\uparrow,} H], C_{q\uparrow}^{+} \rangle\rangle \quad (4)$$

Now evaluating the commentator $[C_{q\uparrow}, H]$, using the Hamiltonian equation (2)

We get the commutative between $C_{q\uparrow}$ and H which is defined as follows

$$[C_{q\uparrow}, H] = \sum_{k\sigma} \epsilon_k C_{k\sigma}^{+} C_{k\sigma} - \sum_{kk'\sigma\sigma\prime} (V_s - U) C_{k\sigma}^{+} C_{-k\sigma\prime}^{+} C_{-k\prime\sigma\prime} C_{k\prime\sigma} - \sum_{k\sigma} \frac{V_P}{2} C_{k\sigma}^{+} C_{k\sigma} \quad (5)$$

Putting value of commutator $[C_{q\uparrow,} H]$ in the equation (4) , $\omega G_{qq}^{\uparrow\uparrow} = \frac{1}{2\pi} + \ll [C_{q\uparrow,} H], C_{q\uparrow}^{+} \gg$

After solving

$$\omega G_{qq}^{\uparrow\uparrow} = \frac{1}{2\pi} + \langle\langle \epsilon_q C_{q\uparrow} C_{q\uparrow}^{+} \rangle\rangle - \sum_{k\prime} (V_s - U) \langle\langle C_{-q\downarrow}^{+} C_{q\uparrow}^{+} \rangle\rangle \langle C_{-k\prime\uparrow} C_{k\prime\uparrow} \rangle - \frac{V_p}{2} \langle\langle C_{q\uparrow} C_{q\uparrow}^{+} \rangle\rangle \quad (6)$$

Now we introduce the order parameter Δ such as

$$\Delta = \sum_{k\prime} (V_s - U) \langle C_{-k\prime\downarrow} C_{k\prime\uparrow} \rangle$$

Substituting above order parameter in equation (6) finally we obtained the equation

$$\left(\omega - \epsilon_q + \frac{V_p}{2}\right) G_{qq}^{\uparrow\uparrow} = \frac{1}{2\pi} - \Delta G_{-qq}^{\uparrow\downarrow} \quad (7)$$

where $G_{-qq}^{\downarrow\uparrow}$ is another Green's function which may be written as

$$G_{-qq}^{\downarrow\uparrow} = \langle\langle C_{-q\downarrow}^{+} C_{q\uparrow}^{+} \rangle\rangle \quad (8)$$

This green's function also may be written in term of equation of motion as

$$\omega G_{-qq}^{\downarrow\uparrow} = \langle\langle [C_{-q\downarrow}^{+}, H], C_{q\uparrow}^{+} \rangle\rangle \quad (9)$$

Evaluating the commentator $[C_{-q\uparrow}^{+} \ H]$, Using the Hamiltonian equation (2) finally obtained equations

$$\left((\omega + \epsilon_q) - \frac{V_P}{2}\right) G_{-qq}^{\downarrow\uparrow} = -\Delta G_{qq}^{\uparrow\uparrow} \quad (10)$$

Now, by the help of equation (7) and equation (10) , We obtain both Green's functions $G_{qq}^{\uparrow\uparrow}$ & $G_{-qq}^{\downarrow\uparrow}$ as

$$G_{-qq}^{\downarrow\uparrow}(\omega) = -\frac{\Delta}{\pi} \frac{1}{\left[\omega^2 - \left(\epsilon_q - \frac{V_P}{2}\right)^2 - \Delta^2\right]} \quad (11)$$

Function replace (ω) in term $(\omega + i \in)$ And $(\omega - i \in)$ then get $G_{-qq}^{\downarrow\uparrow}(\omega + i\epsilon) and G_{-qq}^{\downarrow\uparrow}(\omega - i\epsilon)$ then correlation function

$$\langle C_{-q\downarrow} \ C_{q\uparrow} \rangle = -\frac{1}{i} \int_{-\infty}^{\infty} \frac{G_{-qq}^{\downarrow\uparrow}(\omega + i\in) - G_{-qq}^{\downarrow\uparrow}(\omega - i\in)}{e^{\frac{\omega}{kT}} - \eta} \quad (12)$$

where $\eta = -1$,for formion ,K = Boltzmann constant and T= Temperature , after solving we get correlation function

$$\langle C_{-q\downarrow} \ C_{q\uparrow} \rangle = \sum_k \frac{1}{2} \frac{\Delta}{\sqrt{\left(\epsilon_q - \frac{V_P}{2}\right)^2 + \Delta^2}} \tanh \frac{\sqrt{\left(\epsilon_q - \frac{V_P}{2}\right)^2 + \Delta^2}}{2kT} \quad (13)$$

where $\Delta = \sum_k (V_s - U) \langle C_{-q\downarrow} C_{q\uparrow} \rangle$ Then we can obtained the expression of superconducting order parameter Δ

$$1 = \sum_k (V_s - U) \frac{1}{2} \frac{1}{\sqrt{\left(\epsilon_q - \frac{V_p}{2}\right)^2 + \Delta^2}} \frac{\tanh \sqrt{\left(\epsilon_q - \frac{V_p}{2}\right)^2 + \Delta^2}}{2KT} \quad (14)$$

Converting summation over k' into integration with cut-off energy $\pm\hbar\omega_D$ From the Fermi level, we get

$$1 = N_o(V_s - U) \int_0^{\hbar\omega_D} \frac{1}{\sqrt{\left(\epsilon_q - \frac{V_p}{2}\right)^2 + \Delta^2}} \frac{\tanh \sqrt{\left(\epsilon_q - \frac{V_p}{2}\right)^2 + \Delta^2}}{2KT} d\epsilon_q \quad (15)$$

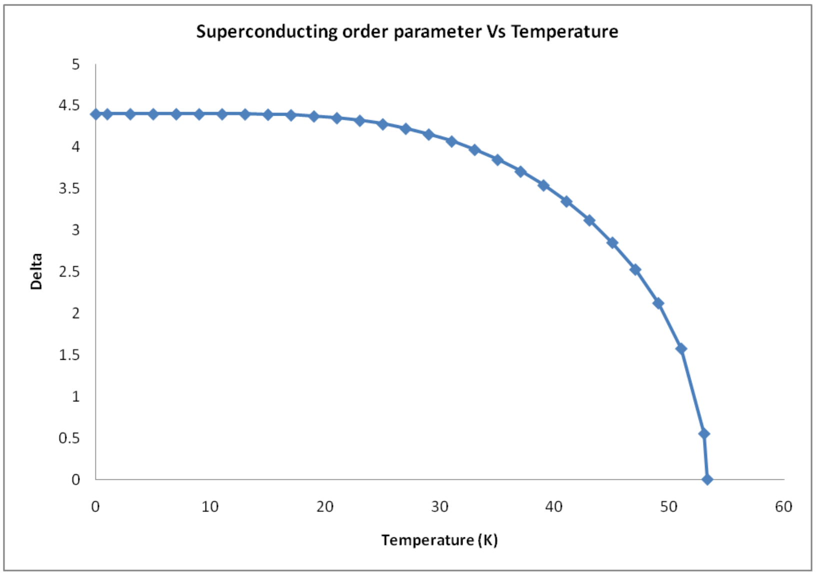
when $\Delta = 0$ *and* $T = Tc$ Then we get

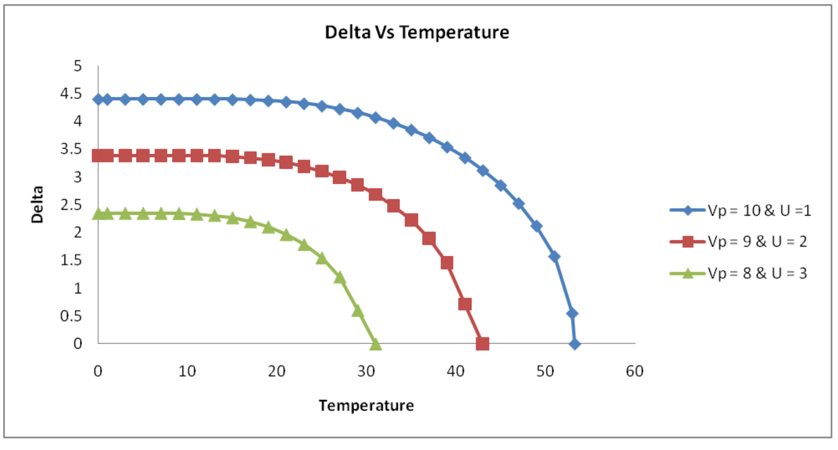
$$1 = N_o(V_s - U) \int_0^{\hbar\omega_D} \frac{1}{\sqrt{\left(\epsilon_q - \frac{V_p}{2}\right)^2}} \frac{\tanh \sqrt{\left(\epsilon_q - \frac{V_p}{2}\right)^2}}{2KTc} d\epsilon_q \quad (16)$$

After calculating, Transition temperature

$$Tc = 1.13072 \frac{\hbar\omega_D}{K_B} e^{-\frac{1}{N_O(V_S - U)}} \quad (17)$$

By using equation(15)&(17), we numerically calculated superconducting order parameter and transition temperature for defferent values of V_p .





Results and Discussion

The first curve represents the variation of superconducting order parameter with temperature (T) for the compound ($LaFeAsO_{1-X}F_X$), x=0.082. curve shows that as increasing the temperature [T] the superconducting order parameter (Δ) decreases and reach to zero at transition temperature [Tc]=53.28K . Second curve is plotted between the temperature (T) and superconducting order parameter (Δ) for different value of electronic polarization (V_p) in As-ions. The upper most curves is for $V_P = 10$ev, the middle one is for $V_p = 9$ev and the lowest is for $V_p = 8$ev . The curve shows that as increasing the V_p the superconducting order parameter as well as transition temperature of the superconductor increases. Hence the electronic polarization V_p helps to stabiles superconducting order and increase the transition temperature Tc .

Conclusion

we can say that the electronic polarization V_p plays an important role to increase transition temperature Tc and help to maintain superconducting order in iron-pitied superconductor.

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