The two band model for iron pnictide based superconductors is used in present work. Using Green’s function technique and equation of motion method, we have obtained expression for superconducting order parameter, Transition temperature, Density of state and Electronic Specific Heat. The theoretical results are then applied to LiFeAs superconductor and comparison with experimental results are made. It is found that the jump in specific heat at $T_c$ is ..., which is very close to the experimental value…. The two gap and $T_c$ are obtained which have good agreement with the experimental results. Further it is also found that interband interaction has positive effect on $T_c$.

KEYWORDS: Iron pnictides superconductors, Multiband superconductors, Transition temperature($T_c$), Density of State, Electronic Specific Heat.
compounds. Role of interband and intraband interactions has been emphasized for enhancement of superconducting Transition temperature ($T_c$)[9] and other superconducting properties. The compound, which has been studied in this article is LiFeAs. It belongs to 111 family of iron pnictide superconductors. The crystal structure is very simple. It contains a layer of arsenic sandwiched between a layer of lithium and a layer of iron. In this work electronic specific heat, critical temperature and density of states is calculated theoretically using Green’s function technique.

**MATHEMATICAL FORMULATIONS**

The Hamiltonian for our system is described as[10]

$$
H = \sum_{\mathbf{k}\sigma} \epsilon_{qs} C_{qs}^+ C_{qs} - \sum_{\mathbf{K}} V_{ss} C_{K\uparrow}^+ C_{K\uparrow} C_{K\uparrow} C_{K\uparrow} + \sum_{\mathbf{k}\sigma} \epsilon_{sd} d_{sd}^+ d_{sd} - \sum_{\mathbf{k}} V_{sd} d_{sd}^+ d_{sd}^+ d_{sd}^+ + \sum_{\mathbf{k}\sigma} (\epsilon_{sd} - \epsilon_{qs}) C_{qs}^+ c_{qs} + \hbar \sum_{\mathbf{k}\sigma} (c_{qs}^+ d_{sd} + d_{sd}^+ c_{qs}) 
$$

(1)

Where, First term denotes the energy of free electrons in p-band, second term denotes the interaction energy of cooper pairs in same layer in p-band of LiFeAs. Third term denotes the energy of free electrons in d-band, fourth term denotes the interaction energy of cooper pairs in same layer in d-band of LiFeAs. Fifth term denotes the interlayer interaction between ‘p’ and ‘d’ bands of LiFeAs and sixth term denotes the hopping term of LiFeAs.

In the present work double time retarded Green’s function technique has been used as mathematical tools for investigation of superconducting transition temperature, density of state, electronic specific heat and order parameter ($\Delta$) taking interlayer interaction between LiFeAs layers.

Now evaluating the commutator $\langle C_{q\uparrow}, C_{q\uparrow}^+ \rangle$, we get

$$
\omega \ll C_{q\uparrow}, C_{q\uparrow}^+ \Rightarrow \frac{1}{2} [C_{q\uparrow}, C_{q\uparrow}^+] + [H, C_{q\uparrow}^+] = \frac{1}{2} \frac{\omega \hbar}{2\pi} G_1 + (\Delta_s + \frac{V_{ss} V_{dd}}{V_{sd}}) G_2 + (V_{sd} \theta_{11} - \frac{\omega \hbar}{2\pi}) G_7 = 0
$$

Similarly writing equation of motion for other Green’s function, we get

$$
(\omega + \epsilon_{qs}) G_1 + (\Delta_s + \frac{V_{sd} V_{dd}}{V_{ss}}) G_4 + (V_{sd} \theta_{11} + h) G_8 = 0
$$

$$
(\omega + \epsilon_{qs}) G_3 + (\Delta_s + \frac{V_{sd} V_{dd}}{V_{ss}}) G_4 + (V_{sd} \theta_{11} - h) G_5 = 0
$$

$$
(\omega + \epsilon_{qs}) G_4 + (\Delta_s + \frac{V_{sd} V_{dd}}{V_{ss}}) G_5 + (V_{sd} \theta_{11} - h) G_6 = 0
$$

$$
(\omega - \epsilon_{qs}) G_5 + (\Delta_s + \frac{V_{sd} V_{dd}}{V_{ss}}) G_6 + (V_{sd} \theta_{11} - h) G_3 = \frac{1}{2\pi}
$$

$$
(\omega - \epsilon_{qs}) G_6 + (\Delta_s + \frac{V_{sd} V_{dd}}{V_{ss}}) G_7 + (V_{sd} \theta_{11} + h) G_4 = 0
$$

$$
(\omega - \epsilon_{qs}) G_7 + (\Delta_s + \frac{V_{sd} V_{dd}}{V_{ss}}) G_8 + (V_{sd} \theta_{11} - h) G_1 = 0
$$

$$
(\omega + \epsilon_{qs}) G_1 + (\Delta_s + \frac{V_{sd} V_{dd}}{V_{ss}}) G_4 + (V_{sd} \theta_{11} - h) G_5 = 0
$$

$$
(\omega - \epsilon_{qs}) G_2 + (\Delta_s + \frac{V_{sd} V_{dd}}{V_{ss}}) G_5 + (V_{sd} \theta_{11} - h) G_8 = 0
$$

$$
(\omega + \epsilon_{qs}) G_4 + (\Delta_s + \frac{V_{sd} V_{dd}}{V_{ss}}) G_7 + (V_{sd} \theta_{11} + h) G_2 = 0
$$

and substituting the value of equation (2) in above solved commutators we get equations of motion as

1. \begin{align*}
(\omega + \epsilon_{qs}) G_1 + \Delta_s G_2 + (V_{ss} \theta_{11} - \frac{\omega \hbar}{2\pi}) G_7 = \frac{1}{2\pi}
\end{align*}

2. \begin{align*}
(\omega + \epsilon_{qs}) G_2 + \Delta_s G_1 + (V_{ss} \theta_{11} + h) G_8 = 0
\end{align*}

3. \begin{align*}
(\omega - \epsilon_{qs}) G_3 + \Delta_s G_4 + (V_{ss} \theta_{11} - h) G_5 = 0
\end{align*}

4. \begin{align*}
(\omega + \epsilon_{qs}) G_4 + \Delta_s G_3 + (V_{ss} \theta_{11} + h) G_6 = 0
\end{align*}

5. \begin{align*}
(\omega - \epsilon_{qs}) G_5 + \Delta_s G_6 + (V_{ss} \theta_{11} - h) G_3 = \frac{1}{2\pi}
\end{align*}

6. \begin{align*}
(\omega - \epsilon_{qs}) G_6 + \Delta_s G_5 + (V_{ss} \theta_{11} + h) G_4 = 0
\end{align*}

7. \begin{align*}
(\omega - \epsilon_{qs}) G_7 + \Delta_s G_8 + (V_{ss} \theta_{11} - h) G_1 = 0
\end{align*}

8. \begin{align*}
(\omega + \epsilon_{qs}) G_8 + \Delta_s G_7 + (V_{ss} \theta_{11} + h) G_2 = 0
\end{align*}
Order parameters

Solving equations of motion we get green’s function
\[
G_2 = \frac{\Delta_1}{2\pi(\Delta_2^2 - \omega^2 + \epsilon_d^2)}
\]
\[
G_6 = \frac{\Delta_2}{2\pi(\Delta_2^2 - \omega^2 + \epsilon_d^2)}
\]

Using green’s function, we obtain the expression for order parameter
\[
\Delta_e = v_{ss} < C_{k+1}^+ C_{-k+1}^- > \ldots (3)
\]

The correlation parameter \( < C_{k+1}^+ C_{-k+1}^- > \) is related to green function \( G_2 \) as -
\[
< C_{k+1}^+ C_{-k+1}^- > = \frac{1}{i} \int_{-\infty}^{\infty} \frac{\Delta_1(\omega^2 + \epsilon^2)}{\omega^2 - E_s^2} \, d\omega \ldots (4)
\]

Where \( \eta = -1 \) for fermions, \( K = \text{Boltzmann constant} \) & \( T = \text{Temperature} \).

Substituting the values of both green’s function we get:
\[
< C_{k+1}^+ C_{-k+1}^- > = \frac{\Delta_1}{2} \tanh \frac{\sqrt{\Delta_1^2 + E_s^2 / 2KT}}{\sqrt{\Delta_1^2 + \epsilon_d^2}}
\]

Solving above equation we get---
\[
< C_{k+1}^+ C_{-k+1}^- > = \frac{\Delta_1}{2} \tanh \frac{\sqrt{\Delta_1^2 + E_s^2 / 2KT}}{\sqrt{\Delta_1^2 + \epsilon_d^2}}
\]

Thus we substitute the above value in equation (4) and obtain the expression of order parameter
\[
\Delta_e = \sum \frac{\Delta_1 v_{ss}}{2} \tanh \frac{\sqrt{\Delta_1^2 + E_s^2 / 2KT}}{\sqrt{\Delta_1^2 + \epsilon_d^2}}
\]

And similarly for d- band
\[
\Delta_d = \sum \frac{\Delta_2 v_{dd}}{2} \tanh \frac{\sqrt{\Delta_2^2 + E_d^2 / 2KT}}{\sqrt{\Delta_2^2 + \epsilon_d^2}}
\]

Transition temperature:

Converting summation into integration we get:
\[
\Delta_e = \frac{\Delta_1 \varepsilon_s N_s}{2} \int_0^{\hbar \omega_d} \frac{\sqrt{\Delta_1^2 + \epsilon_s^2 / 2KT}}{\sqrt{\Delta_1^2 + \epsilon_d^2}} \, d\epsilon_d
\]

following Shul et. al. [11] and Priyanshu[12], we calculated
\[
\Delta_e = v_{ss} \Delta_1 N_s F(A) \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots (5)
\]

Similarly we get…..
\[
\Delta_d = v_{dd} \Delta_2 N_d F(B) \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots (6)
\]

Now on adding and subtracting \( v_{dd} \Delta_d \) from equation (5) and comparing it with (6) we get:
\[
A[1 - V_{ss}N_s F(A)] = v_{sd} BN_d F(B) \ldots (7)
\]

Now on adding and subtracting \( v_{dd} \Delta_d \) from equation (6) and comparing it with (5) we get:
\[
B[1 - V_{dd}N_d F(B)] = v_{sd} AN_s F(A) \ldots (8)
\]

Now multiply (7) and (8), we get-
\[
[v_{sd}^2 N_s N_d - v_{ss} v_{dd} N_s N_d] F(A) F(B) + v_{dd} N_d F(A)
\[
+ v_{sd} N_s F(B) - 1]
\]

When \( T = T_c \) , and \( A, B = 0 \), above equation may be written as-
\[
[v_{sd}^2 N_s N_d - v_{ss} v_{dd} N_s N_d] F(0) + v_{dd} N_d F(0) - 1]
\]

Dividing above equation by \( N_s N_d \) and solving for \( F(0) \) we get-

Density of state

The density of state is an important function which has important role in interlayer interaction. The density of state (DOS) of a system describes the number of states per interval of energy at each energy level that are available to be occupied.

For density of state again we solve equation motion for green’s function \( G_1 \) and \( G_5 \)

\[
G_1 = \frac{(\omega + \epsilon_0)}{2\pi(\Delta_2^2 - \omega^2 + \epsilon_0^2)}
\]

\[
G_5 = \frac{(\omega + \epsilon_0)}{2\pi(\Delta_2^2 - \omega^2 + \epsilon_0^2)}
\]

The density of state per atom \( N(\omega) \) is defined as:

\[
N_s(\omega) = \lim_{\epsilon \to 0} \sum_{s}[G_1(s, \omega + i\epsilon) - G_1(s, \omega - i\epsilon)]
\]

Where, \( N_s(\omega) \) is the density of state function for p-band.

For d-band we have ----

\[
N_d(\omega) = \lim_{\epsilon \to 0} \sum_{d}[G_5(d, \omega + i\epsilon) - G_5(d, \omega - i\epsilon)]
\]

Where, \( G_1 \) is one particle green function for s-band is

\[
\ll C_q^+, C_q^- \gg = \frac{\epsilon_q}{(\omega^2 - E_q^2 - \epsilon_q)}
\]

Where \( E_q^2 = \epsilon_q^2 + \Delta_4^2 \)

Solving equation (9) by partial fraction method, we obtain

\[
\ll C_q^+, C_q^- \gg = \frac{1}{2} \left[ \frac{1}{(\omega - E_q)} + \frac{1}{(\omega + E_q)} \right] + \frac{\epsilon_q}{2 E_q} \left( \frac{1}{(\omega - E_q)} - \frac{1}{(\omega + E_q)} \right)
\]

Now

\[
\frac{I}{\epsilon - \omega} \frac{1}{2\pi N} \left( \frac{1}{(\omega - E_q)} - \frac{1}{(\omega + E_q)} \right) = \delta(\omega - E_q)
\]

substituting this values in equation (10) we get:

\[ N_s(\omega) = \frac{1}{2} \sum_{\alpha} [(1 + \frac{\omega}{E_{\alpha}}) \delta(\omega - E_{\alpha}) + (1 - \frac{\omega}{E_{\alpha}}) \delta(\omega + E_{\alpha})] \]……………………..(15)

If \( \omega = E_{\alpha} \)

Changing summation into integration we get:

\[ N_s(\omega) = N_s(0) \int (1 + \frac{\omega}{E_{\alpha}}) d\omega \]……………………..(16)

\[ \frac{N_s(\omega)}{N_s(0)} = \int (1 + \frac{\omega}{E_{\alpha}}) d\omega \]……………………..(17)

After simplification, we obtain the expression for density of state for p-band,

\[ \frac{N_s(\omega)}{N_s(0)} = \begin{cases} 2 \frac{\omega}{\sqrt{\omega^2 - \Delta_p^2}} & \text{for } \omega > 0 \\ 0 & \text{otherwise} \end{cases} \]……………………..(18)

Similarly we get expression for density of state for d-band, that is –

\[ \frac{N_d(\omega)}{N_d(0)} = \begin{cases} 2 \frac{\omega}{\sqrt{\omega^2 - \Delta_d^2}} & \text{for } \omega > 0 \\ 0 & \text{otherwise} \end{cases} \]……………………..(19)

**Specific heat**

Calculating the correlation function \( \langle C_{k1}^+, C_{k1} \rangle \) and this is related to Green’s function \( G_1 \).

Where,

\[ \langle C_{k1}^+, C_{k1} \rangle = -\frac{1}{\pi} \int_{-\infty}^{\infty} \frac{\omega + E_{\alpha}}{\omega^2 - E_{\alpha}^2} d\omega \]……………………..(20)

Where, \( \eta = -1 \) for fermions and Boltzmann constant and \( T = \) Temperature. Substituting the value in equation (17) we get:

\[ \langle C_{k1}^+, C_{k1} \rangle = -\frac{1}{\pi} \int_{-\infty}^{\infty} \frac{\omega + E_{\alpha}}{\omega^2 - E_{\alpha}^2} d\omega \]

\[ \langle C_{k1}^+, C_{k1} \rangle = \frac{\omega + E_{\alpha}}{2} tanh \frac{\Delta_{k1}^2 + E_{\alpha}^2}{2kT} \]

Electronic specific heat for S band from above correlation function is given as:

\[ C_{es}^s = \frac{d}{dT} \frac{1}{N} \int 2E_s < C_{k1}^+, C_{k1} > \]

\[ C_{es}^s = \frac{1}{N} \int 2E_s \frac{\omega + E_{\alpha}}{2} tanh \frac{\Delta_{k1}^2 + E_{\alpha}^2}{2kT} \]

Now converting the summation over \( s \) into a integration with cutoff energy +h\( \omega_o \) from the Fermi level, we get:

\[ C_{es}^s = \frac{2}{NkT^2} \int_0^{h\omega_o} \frac{\omega}{\sqrt{\omega^2 - \Delta_{k1}^2}} d\omega \]……………………..(21)

Similarly we get the expression for electronic specific heat for d-band

\[ C_{es}^d = \frac{2}{NkT^2} \int_0^{h\omega_o} \frac{\omega}{\sqrt{\omega^2 - \Delta_{d1}^2}} d\omega \]……………………..(22)

**RESULT AND CONCLUSION**

In above study, we have calculated various thermodynamical properties of a two-band LiFeAs superconductor with the help of BCS Hamiltonian containing p and d-bands[13-14]. Using the Green’s function technique and equation of motion, we obtained the expressions for superconducting order parameters \( \Delta_p \) and \( \Delta_d \). Using these order parameters and other available experimental data, following observations were made.

1. The transition temperature for above mentioned LiFeAs system has numerically been calculated as 18K[15] with \( \alpha = \left( \frac{v_{dd}}{N_s} + \frac{v_{ss}}{N_d} \right) \). Figure (1) below shows variation of transition temperature for iron pnictides superconductors with average interaction energies resulting from phonon emission and absorption by p, d-band process. It shows that transition temperature increases with interband interaction \( V_{dd} \). As it can be seen from equation (9), h\( \omega_o \) corresponds to phonon frequency, another term \( e^{\alpha} \) is collectively
responsible for increasing $T_c$ [16,17]. For numerical calculations $\hbar \omega = 0.24eVÅ$[18].

Figure:-1

Variation of transition temperature with respect to average interaction energy.

2. The density of state (DOS)[19,20] behaviour is similar to BCS weak coupling. Figure (2) below corresponding to p and d-band, there is marked difference between the two curves. This reveals LiFeAs superconductors differ from conventional metallic superconductor. This is the major difference between the two classes of superconductors and may be partly responsible for the differences in their properties. It is noted that the density of state for the system LiFeAs is quite high.

Figure:-2

Variation of density of states function with $\omega$ for both p-bands and d-bands

3. Using the above values of $\Delta_p$ and $\Delta_d$ we calculated $\Delta_1$ and $\Delta_2$. Using these $\Delta_1$ and $\Delta_2$ and other relevant experimental values for the reference we calculated the value of electronic specific heat for both p and d-bands and got the expressions as mentioned in equations (21) and (22).

The term $\hbar \omega_D$ represents the phonon frequency and its value is 0.24eVÅ[18]. K is the Boltzmann constant and its value is $8.632X10^{-5}eV/K$. N is the density of states. The Transition temperature of the compound LiFeAs is 18K. Figure (3) shows the variation of specific heat with the temperature. We can see a drop in specific heat at the transition temperature. The drop in $\Delta c/T$ for p-band is $1.3906X10^{11}eV/molK^2$ and for d-band is $2.635 X 10^{11}eV/molK^2$ and the experimental result is $4.78 X 10^{16}eV/molK^2$ [21], to $7.75X10^{16}eV/molK^2$ [3], $\approx$ to $12.5 X 10^{16}eV/molK^2$ [22].
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