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THERMODYNAMICAL PROPERTIES OF LiFeAs SUPERCONDUCTOR USING TWO BAND MODEL

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ABSTRACT

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 comparision 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.

INTRODUCTION

Soon after the discovery of high temperature superconductivity in class of iron pnictides in February 2008, various studies of the parent compound have revealed a perspective of these exciting materials that is far richer than previously anticipated. While in the early days the techniques used to understand these compounds seemed sufficient, several recent studies suggest that understanding the vast physics of these materials may require more advanced concepts.

The main speciality of iron-pnictide superconductors is their multiband nature. The multiple bands at the Fermi surface suggest the possibility for multi-band superconductivity in this class of superconductors. It is found that the Fermi surfaces of these compounds consist of several holes and electron-like cylinders [1]. Further it is also found that these compounds have multi-energy gaps as well [2-3]. Phonon interaction alone is not sufficient enough to explain the high critical temperature (T_c). In several theoretical studies, the multiband superconductivity is stated as a possible explanation for the high critical temperature (T_c)[4]. Indeed, it is well known that

multiband effects can strongly enhance the superconductivity [5]. This is particularly true in the case of iron pnictides. Another advantage of this mechanism is that the interband interaction can enhance superconductivity irrespective of whether it is attractive or repulsive provided that the gaps in different bands have the same or opposite signs, respectively. In such multiple band systems intraband coupling is provided by phonons while interband coupling by any other mechanism[6].

It is natural to describe an iron pnictide superconductor by means of a two band model with interband and intraband coupling as angle resolved photoemission spectroscopy(ARPES) experiments show that Fermi surface consists almost cylindrical hole and electron pockets respectively. An itinerant model of electron pockets and holes Fermi surface shows that the same interaction, inter-band hopping, induces a spin-density-wave order and superconductivity[7-8].

Various studies incorporating layered structure throw light on the unusual properties of the pnictide

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]

$H = \sum_{k\sigma} \in_{qs} C_{K\sigma}^+ C_{K\sigma} - \sum_{KK'} V_{SS} C_{K\uparrow}^+ C_{-K\downarrow}^+ C_{-K'\downarrow} C_{K'\uparrow} + \sum_{K\sigma} \in_{kd} d_{k\sigma}^+ d_{k\sigma} - \sum_{kk'} V_{dd} d_{k\uparrow}^+ d_{k\downarrow}^+ d_{-k'\downarrow} d_{k'\uparrow} - \sum_{kk'} V_{sd} (c_{k\uparrow}^+ c_{-k\downarrow}^+ d_{-k'\downarrow} d_{k'\uparrow} + d_{k\uparrow}^+ d_{-k\downarrow}^+ c_{-k'\downarrow} c_{k'\uparrow}) + h \sum_{k\sigma} \{c_{k\sigma}^+ d_{k\sigma} + d_{k\sigma}^+ c_{k\sigma}\}$ ...(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 trantition temperature, density of state , electronic specific heat and order parameter (Δ) taking interlayer interaction between LiFeAs layers.

Now evaluating the commutator $<C_{q\uparrow}, C_{q\uparrow}^{\dagger}>$, we get
$\omega \ll C_{q\uparrow}, C_{q\uparrow}^+ \gg = \frac{1}{2\pi} [C_{q\uparrow}, C_{q\uparrow}^+]_\eta + \ll [C_{q\uparrow}, H], C_{q\uparrow}^+ \gg$
$(\omega - \varepsilon_{qs})G_1 + \left(\Delta_s + \frac{V_{sd}}{V_{dd}}\Delta_d\right) G_2 + (V_{sd}\vartheta_{\downarrow\downarrow} - h)G_7 = \frac{1}{2\pi}$

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

$(\omega + \varepsilon_{-qs})G_2 + \left(\Delta_s + \frac{V_{sd}}{V_{dd}}\right) G_1 + (V_{sd}\vartheta_{\uparrow\uparrow} + h)G_8 = 0$

$(\omega - \varepsilon_{qs})G_3 + \left(\Delta_s + \frac{V_{sd}}{V_{dd}}\Delta_d\right) G_4 + (V_{sd}\vartheta_{\downarrow\downarrow} - h)G_5 = 0$

$(\omega + \varepsilon_{-qs})G_4 + \left(\Delta_s + \frac{V_{sd}}{V_{dd}}V_d\right) G_3 + (V_{sd}\vartheta_{\uparrow\uparrow} - h)G_6 = 0$

$(\omega - \varepsilon_{qd})G_5 + \left(\Delta_d + \frac{V_{sd}}{V_{ss}}\Delta_s\right) G_6 + (V_{sd}\vartheta_{\downarrow\downarrow} - h)G_3 = \frac{1}{2\pi}$

$(\omega + \varepsilon_{-qd})G_6 + \left(\Delta_d + \frac{V_{sd}}{V_{ss}}\Delta_s\right) G_5 + (V_{sd}\vartheta_{\uparrow\uparrow} + h)G_4 = 0$

$(\omega - \varepsilon_{qd})G_7 + \left(\Delta_d + \frac{V_{sd}}{V_{ss}}\Delta_s\right) G_8 + (V_{sd}\vartheta_{\downarrow\downarrow} - h)G_1 = 0$

$(\omega + \varepsilon_{-qd})G_8 + \left(\Delta_d + \frac{V_{sd}}{V_{ss}}\Delta_s\right) G_7 + (V_{sd}\vartheta_{\uparrow\uparrow} + h)G_2 = 0$

where

$\left(\Delta_s + \frac{V_{sd}}{V_{dd}}\Delta_d\right) = \Delta_1$
$\left(\Delta_d + \frac{V_{sd}}{V_{ss}}\Delta_s\right) = \Delta_2$

$\left.\right\}$ (2)

And $V_{sd}\vartheta_{\downarrow\downarrow}$ and $V_{sd}\vartheta_{\uparrow\uparrow} = V_r$.

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

1. $(\omega - \varepsilon_{qs})G_1 + \Delta_1 G_2 + (V_r - h)G_7 = \frac{1}{2\pi}$
2. $(\omega + \varepsilon_{-qs})G_2 + \Delta_1 G_1 + (V_r + h)G_8 = 0$
3. $(\omega - \varepsilon_{qs})G_3 + \Delta_1 G_4 + (V_r - h)G_5 = 0$
4. $(\omega + \varepsilon_{-qs})G_4 + \Delta_1 G_3 + (V_r + h)G_6 = 0$
5. $(\omega - \varepsilon_{qd})G_5 + \Delta_2 G_6 + (V_r - h)G_3 = \frac{1}{2\pi}$
6. $(\omega + \varepsilon_{-qd})G_6 + \Delta_2 G_5 + (V_r + h)G_4 = 0$
7. $(\omega - \varepsilon_{qd})G_7 + \Delta_2 G_8 + (V_r - h)G_1 = 0$
8. $(\omega + \varepsilon_{-qd})G_8 + \Delta_2 G_7 + (V_r + h)G_2 = 0$

Order parameters

Solving equations of motion we get green's function

$$G_2 = \frac{\Delta_1}{2\pi(\Delta_2^2 - \omega^2 + \bar{\varepsilon}_s^2)}$$

$$G_6 = \frac{\Delta_2}{2\pi(\Delta_2^2 - \omega^2 + \bar{\varepsilon}_d^2)}$$

Using geen's function, we obtain the expression for order parameter

$$\Delta_s = v_{ss} < C_{k\uparrow}^+, C_{-k\downarrow}^+ > \quad ...(3)$$

The correlation parameter $< C_{k\uparrow}^+, C_{-k\downarrow}^+ >$ is related to green function G_2 as -

$$< C_{k\uparrow}^+, C_{-k\downarrow}^+ > = -\frac{1}{i} \int_{-\infty}^{+\infty} \frac{G_2(s,\omega+i\varepsilon) - G_2(s,\omega-i\varepsilon)}{e^{\omega/KT} - \eta} d\omega \quad ...(4)$$

Where $\eta = -1$ for fermions, K=Boltzmann constant & T= Temperature.

Substituting the values of both green's function we get:

$$< C_{k\uparrow}^+, C_{-k\downarrow}^+ > = -\frac{1}{i} \int_{-\infty}^{+\infty} \frac{\Delta_1(\omega^2 + \varepsilon^2)}{\omega^2 - E_s{}^2} d\omega$$

Solving above equation we get---

$$< C_{k\uparrow}^+, C_{-k\downarrow}^+ > = \frac{\Delta_1}{2} tanh \frac{\sqrt{\Delta_1^2 + \bar{\varepsilon}_s^2/2KT}}{\sqrt{\Delta_1^2 + \bar{\varepsilon}_s^2}}$$

Thus we substitute the above value in equation (4) and obtain the expression of order parameter

$$\Delta_s = \sum \frac{\Delta_1 v_{ss}}{2} tanh \frac{\sqrt{\Delta_1^2 + \bar{\varepsilon}_s^2/2KT}}{\sqrt{\Delta_1^2 + \bar{\varepsilon}_s^2}}$$

And similarly for d- band

$$\Delta_d = \sum \frac{\Delta_2 v_{dd}}{2} tanh \frac{\sqrt{\Delta_2^2 + \bar{\varepsilon}_d^2/2KT}}{\sqrt{\Delta_2^2 + \bar{\varepsilon}_d^2}}$$

Transition temperature:

Converting summation into integration we get:

$$\Delta_s = \frac{\Delta_1}{2} v_{ss} N_s \int_0^{\hbar\omega_d} \frac{\sqrt{\sqrt{\Delta_1^2 + \bar{\varepsilon}_s^2/2KT}}}{\sqrt{\Delta_1^2 + \bar{\varepsilon}_s^2}} d\bar{\varepsilon}_s$$

following Shul *et. al.* [11] and Priyanshu[12], we calculated

$$\Delta_s = v_{ss}\Delta_1 N_s F(A) \quad ....(5)$$

Where, $\int_0^{\hbar\omega_d} \frac{\sqrt{\sqrt{\Delta_1^2 + \frac{\bar{\varepsilon}_s^2}{2KT}}}}{\sqrt{\Delta_1^2 + \bar{\varepsilon}_s^2}} d\bar{\varepsilon}_s = F(A)$

Similarly we get.....

$$\Delta_d = v_{dd}\Delta_2 N_d F(B)..............(6)$$

Where, $\int_0^{\hbar\omega_d} tanh \frac{\sqrt{\Delta_2^2 + \bar{\varepsilon}_d^2/2KT}}{\sqrt{\Delta_2^2 + \bar{\varepsilon}_d^2}} d\bar{\varepsilon}_d = F(B)$

Now on adding and subtracting $\frac{v_{sd}}{v_{dd}}\Delta_d$ from equation (5) and compairing it with (6) we get:

$$A[1 - V_{ss}N_s F(A)] = v_{sd} B N_d F(B) \quad ...(7)$$

Now on adding and subtracting $\frac{v_{sd}}{v_{ss}}\Delta_s$ from equation (6) and compairing it with (5) we get:

$$B[1 - V_{dd}N_d F(B)] = v_{sd} A N_s F(A) \quad ...(8)$$

Now multiply (7) and (8), we get-

$$[\{v_{sd}^2 N_s N_d - v_{ss}v_{dd}N_s N_d\}F(A)F(B) + v_{dd}N_d F(A) + v_{ss}N_s F(B) - 1]$$

When T=T$_c$, and A,B=0, above equation may be written as-

$$[\{v_{sd}^2 N_s N_d - v_{ss}v_{dd}N_s N_d\}F^2(0) + \{v_{dd}N_d + v_{ss}N_s\}F(0) - 1]$$

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

$$F(0) = \frac{\frac{1}{4}\left(v_{dd}/N_s + v_{ss}/N_d\right)^2 + (\frac{v_{sd}^2 - v_{ss}v_{dd}}{N_s N_d})^{\frac{1}{2}}}{v_{sd}^2 - v_{ss}v_{dd}}$$
$$- \frac{\frac{1}{2}(v_{dd}/N_s + v_{ss}/N_d)}{v_{sd}^2 - v_{ss}v_{dd}}$$

And therefore –

$$\int_0^{\hbar\omega_d} tanh\frac{\sqrt{\Delta_2^2 + \bar{\varepsilon}_d^2/2KT}}{\sqrt{\Delta_2^2 + \bar{\varepsilon}_d^2}} d\bar{\varepsilon}_d = F(0)$$
$$= log\frac{\hbar\omega}{2KT_c} + 0.08185$$

Hence

$$log\frac{\hbar\omega}{2KT_c} + 0.08185$$
$$= \frac{\frac{1}{4}\left(v_{dd}/N_s + v_{ss}/N_d\right)^2 + (\frac{v_{sd}^2 - v_{ss}v_{dd}}{N_s N_d})^{\frac{1}{2}}}{v_{sd}^2 - v_{ss}v_{dd}}$$
$$- \frac{\frac{1}{2}(v_{dd}/N_s + v_{ss}/N_d)}{v_{sd}^2 - v_{ss}v_{dd}}$$

Or

$$\frac{\hbar\omega}{2KT_c} = e^{(\alpha - 0.8185)}$$

Where,

$$\alpha = \frac{\frac{1}{4}\left(v_{dd}/N_s + v_{ss}/N_d\right)^2 + (\frac{v_{sd}^2 - v_{ss}v_{dd}}{N_s N_d})^{\frac{1}{2}}}{v_{sd}^2 - v_{ss}v_{dd}} - \frac{\frac{1}{2}(v_{dd}/N_s + v_{ss}/N_d)}{v_{sd}^2 - v_{ss}v_{dd}}.$$

$$KT_c = \frac{1}{2}\hbar\omega e^{-\alpha}e^{0.8185}$$

$$KT_c = 1.137\hbar\omega e^{-\alpha}$$

$$KT_c$$
$$= 1.137\hbar\omega \; e^{-\frac{\frac{1}{4}\left(v_{dd}/N_s + v_{ss}/N_d\right)^2 + (\frac{v_{sd}^2 - v_{ss}v_{dd}}{N_s N_d})^{\frac{1}{2}}}{v_{sd}^2 - v_{ss}v_{dd}} - \frac{\frac{1}{2}(v_{dd}/N_s + v_{ss}/N_d)}{v_{sd}^2 - v_{ss}v_{dd}}}$$

Finally T_c may be expressed as-

$$T_c = \frac{1.137\hbar\omega \; e^{\frac{\frac{1}{4}\left(v_{dd}/N_s + v_{ss}/N_d\right)^2 + (\frac{v_{sd}^2 - v_{ss}v_{dd}}{N_s N_d})^{\frac{1}{2}}}{v_{sd}^2 - v_{ss}v_{dd}} - \frac{\frac{1}{2}(v_{dd}/N_s + v_{ss}/N_d)}{v_{sd}^2 - v_{ss}v_{dd}}}}{K}$$

…(9)

Density of state

The density of state is an impotant 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

$$G_1 = \frac{(\omega + \varepsilon_s)}{2\pi(\Delta_2^2 - \omega^2 + \bar{\varepsilon}_s^2)}$$

$$G_5 = \frac{(\omega + \varepsilon_d)}{2\pi(\Delta_2^2 - \omega^2 + \bar{\varepsilon}_d^2)}$$

The density of state per atom N(ω)is defined as-

$$Ns(\omega) = \lim_{\varepsilon \to 0}\sum_s[G_1(s, \omega + i\varepsilon) - G_1(s, \omega - i\varepsilon)]\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots(10)$$

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

For d-band we have ----

$$N_d(\omega) = \lim_{\varepsilon \to 0}\sum_d[G_5(d, \omega + i\varepsilon) - G_5(d, \omega - i\varepsilon)]\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots(11)$$

Where G_1 is one particle green function for s-band is

$$\ll C_{q\uparrow}, C_{q\uparrow}^+ \gg = \frac{(\omega + \overline{\varepsilon_s})}{(\omega^2 - E_s^2)}\dots\dots\dots\dots\dots\dots\dots\dots\dots(12)$$

Where $E_s^2 = \bar{\varepsilon}_s^2 + \Delta_1^2$

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

$$\ll C_{q\uparrow}, C_{q\uparrow}^+ \gg = \frac{1}{2}\left[\frac{1}{(\omega - E_s)} + \frac{1}{(\omega + E_s)}\right] + \frac{\bar{\varepsilon_s}}{2E_s}\left[\frac{1}{(\omega - E_s)} - \frac{1}{(\omega + E_s)}\right]\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots(13)$$

Now

$$\lim_{\varepsilon \to 0}\frac{i}{2\pi N}\left[\frac{1}{(\omega + i\epsilon - E_s)} - \frac{1}{(\omega - i\epsilon - E_s)}\right]$$
$$\cong \lim_{\varepsilon \to 0}\frac{\varepsilon}{\pi N\{(\omega - E_s)^2 - \varepsilon^2\}} = \delta(\omega - E_s) \dots\dots\dots\dots\dots(14)$$

substituting this values in equation (10) we get:

$$N_s(\omega) = \frac{1}{2}\sum_s[(1 + \frac{\bar{\varepsilon}_s}{E_s})\,\delta(\omega - E_s) + (1 - \frac{\bar{\varepsilon}_s}{E_s})\,\delta(\omega + E_s)]\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(15)$$

If $\omega = E_s$

Changing summation into integration we get:

$$N_s(\omega) = N_s(0)\int\left(1 + \frac{\bar{\varepsilon}_s}{\omega}\right)d\omega \ldots\ldots\ldots\ldots\ldots\ldots\ldots(16)$$

$$\frac{N_s(\omega)}{N_s(0)} = \int\left(1 + \frac{\bar{\varepsilon}_s}{\omega}\right)d\omega\ldots\ldots\ldots\ldots\ldots\ldots\ldots(17)$$

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

$$\frac{N_s(\omega)}{N_s(0)} = \begin{cases} 2\frac{\omega}{\sqrt{\omega^2 - \Delta_1^2}} & \text{for } \omega > 0 \\ 0 & \text{otherwise} \end{cases} \ldots\ldots\ldots(18)$$

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

$$\frac{N_d(\omega)}{N_d(0)} = \begin{cases} 2\frac{\omega}{\sqrt{\omega^2 - \Delta_2^2}} & \text{for } \omega > 0 \\ 0 & \text{otherwise} \end{cases} \ldots\ldots\ldots(19)$$

Specific heat

Calculating the correlation function $< C_{k\uparrow}^\dagger, C_{k\uparrow} >$ and this is related to Green's function G_1.

Where,

$$< C_{k\uparrow}^\dagger, C_{k\uparrow} > = -\frac{1}{i}\int_{-\infty}^{\infty}\frac{G_1(\omega + i\varepsilon) - G_1(\omega - i\varepsilon)}{e^{\omega/kT} - \eta}d\omega \quad \ldots\ldots(20)$$

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

$$< C_{k\uparrow}^\dagger, C_{k\uparrow} > = -\frac{1}{i}\int_{-\infty}^{\infty}\frac{(\omega + \bar{\varepsilon}_s)}{\omega^2 - E_s^2}d\omega$$

$$< C_{k\uparrow}^\dagger, C_{k\uparrow} > = \frac{(\omega + \bar{\varepsilon}_s)}{2}tanh\frac{\sqrt{\Delta_1^2 + \bar{\varepsilon}_s^2}}{kT}$$

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

$$C_{es}^s = \frac{\partial}{\partial T}\frac{1}{N}\sum 2E_s < C_{k\uparrow}^\dagger, C_{k\uparrow} >$$

$$C_{es}^s = \frac{\partial}{\partial T}\frac{1}{N}\sum 2E_s\frac{(\omega + \varepsilon_s)}{2}tanh\frac{\sqrt{\Delta_1^2 + \bar{\varepsilon}_s^2}}{2KT}$$

Now converting the summation over s into a integration with cutoff energy $+\hbar\omega_D$ from the Fermi level, we get:

$$C_{es}^s = \frac{2}{NKT^2}\int_0^{\hbar\omega_D}\bar{\varepsilon}_s^2\,sech^2[\frac{\sqrt{\Delta_1^2 + \bar{\varepsilon}_s^2}}{2KT}d\bar{\varepsilon}_s \ldots\ldots\ldots(21)$$

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

$$C_{es}^d = \frac{2}{NKT^2}\int_0^{\hbar\omega_D}\bar{\varepsilon}_d^2\,sech^2[\frac{\sqrt{\Delta_2^2 + \bar{\varepsilon}_d^2}}{2KT}d\bar{\varepsilon}_d \ldots\ldots\ldots(22)$$

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 Δp and Δ_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$_{sd}$). As it can be seen from equation (9), $\hbar\omega$ corresponds to phonon frequency, another term $e^{-\alpha}$ is collectively

responsible for increasing T_c [16,17]. For numerical calculations $\hbar\omega = 0.24\text{eVÅ}$[18].
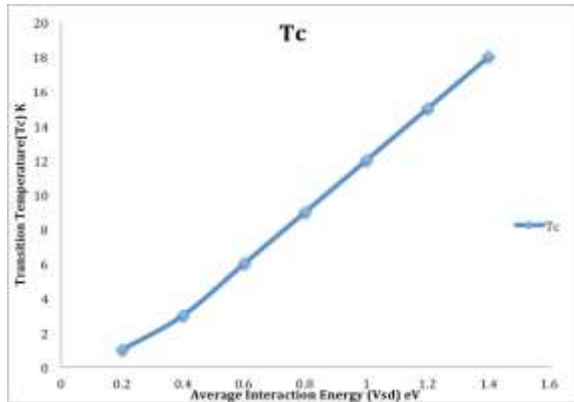
Figure:-1

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
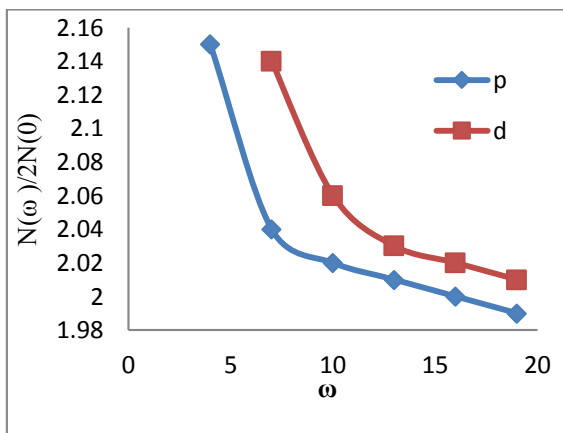
Variation of density of states function with ω for both p-bands and d-bands

3. Using the above values of Δ_p and Δ_d we calculated Δ_1 and Δ_2. Using these Δ_1 and Δ_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 $8.632\text{X}10^{-5}\text{eV/K}$. 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 $1.3906\text{X}10^{11}\text{eV/molK}^2$ and for d-band is $2.635 \text{ X } 10^{11}\text{eV/molK}^2$ and the experimental result is $4.78 \text{ X } 10^{16}\text{eV/molK}^2$ [21], to $7.75\text{X}10^{16}\text{eV/molK}^2$ [3], $\approx$ to $12.5 \text{ X } 10^{16}\text{eV/molK}^2$ [22].

Figure:-3
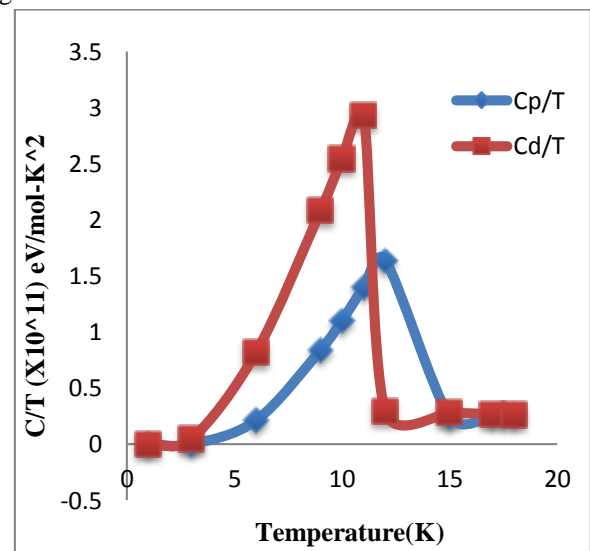
Variation Of Specific Heat with Temperature for both p-band and d-band.

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