

Two band model for the iron based superconductors

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Two band model for Fe-As based oxygen containing superconductors is developed using the Green's function technique and equation of motion method. Self-consistent equations for superconducting order parameters ($\bar{\Delta}_p, \bar{\Delta}_d$), specific heat (C_{es}) and density of states are derived. The theory is applied to explain the experimental results in oxygen containing Fe-As superconductors $\text{Sm}_{0.95}\text{La}_{0.05}\text{O}_{0.85}\text{F}_{0.85}\text{Fe}_{0.15}\text{FeAs}$ and $\text{SmO}_{1-x}\text{F}_x\text{FeAs}$. The comparison to experimental data is given where these are available. The agreement between theory and experiments is quite encouraging.

Keywords: Iron-based superconductors, Green's functions, Density of states, Specific heat

1 Introduction

The recent discovery of high temperature superconductivity in Fe-As based compounds has generated great interest in exploring new high $-T_c$ superconductors and studying the novel superconducting mechanism in these systems¹⁻¹⁵. Up to now, the critical temperature for iron arsenide superconductors has been raised to 57.3 K for $\text{Sm}_{0.95}\text{La}_{0.05}\text{O}_{0.85}\text{F}_{0.85}\text{Fe}_{0.15}\text{FeAs}$ which is the highest for non-cuprate superconductors¹³. Three types of iron arsenide superconductor have been reported so far: (i) '1111' type RFeAsO (R = rare earth metal) (ii) '122' type AeFe_2As_2 (Ae = alkaline earth metal) and (iii) '111' type AFeAs (A = Li, Na). Presently "1111" family based rare-earth oxypnictides RFeAsO (R = La, Sm, Gd, etc.) are in focus of research interest. The T_c 's of the iron based superconductors are too high to be explained by the conventional BCS theory, and have a number of additional features in common with the high $-T_c$ cuprates¹⁶. They contain iron-arsenic (or selenium) layers of atoms, the iron atoms have magnetic moments, the superconductivity is established by Cooper pairs, and the magnetism is known to play a substantial role in the superconducting state. Like the cuprates, the Fe-As based superconductors are highly two dimensional, their parent material¹ shows anti-ferromagnetic long-range order below 150 K and superconductivity occurs upon doping of either electron¹ or holes¹⁴ into Fe-As layers. However, several other properties differ

substantially and promise new interesting physics^{11,17,18}. The undoped 'parent' material in both cases exhibits magnetic order, but the iron-based systems are metals while the cuprates are insulators, which mean that there are fundamental differences in the electronics of these materials. For the cuprates, the Cu and O atoms are in same thin layers, and this renders the superconducting properties highly anisotropic, being very good within the layer and poor along the direction between the layers. In case of Fe-As superconductors, the layers are thick-the As atoms are positioned well off from the plane of iron atoms, and this makes the superconducting properties of these systems much closer to isotropic. The different nature of the anisotropy originate forms a fundamental difference in the pairing for cuprates, the Cooper pairs prefer to be in the CuO planes and are highly anisotropic, while for the Fe-As based superconductors they are almost isotropic. At present the key issues of interest are the effect of various types of doping, pairing mechanism, symmetry of the order parameter, quasi-particle energy spectrum and the superconducting energy gap(s).

All these quaternary rare-earth transition metal arsenide oxides LnOFeAs (Ln=La, Sm, Nd, Pr and Gd) from a tetragonal ZrCuSiAs type layered structure⁹ with the space group $P4/mmm$. The parent compounds were non-superconducting and show anomaly¹³ at about 150 K. The lattice constants of $\text{Sm}_{0.95}\text{La}_{0.05}\text{O}_{0.85}\text{F}_{0.85}\text{Fe}_{0.15}\text{FeAs}$ at room temperature

are: $a = 0.3927$ (Ref.9) nm, and $c = 0.8441(2)$ nm (Ref. 3). Superconductivity emerges at $x=0.10=0.20$. Sample $\text{SmO}_{1-x}\text{F}_x\text{FeAs}_s$ has the maximum superconducting transition temperature has the $T_c(\text{onset})=54$ K. Among the family of $\text{LnO}_{1-x}\text{F}_x\text{FeAs}$ (Ln=La, Sm, Nd, Pr and Gd), specific heat was only studied for $\text{LaO}_{1-x}\text{F}_x\text{Fe}$ compounds so far^{19,64}.

Band structure calculations reveal that the total density of states at the Fermi level $N(0)$ is formed mainly by Fe 3d-states²⁰⁻²². Sadovskii¹⁸ has shown that the T_c values for different iron-based superconductors correlate with $N(0)$, thus giving support to the BCS-like coupling in these compounds. Majority of theories for the pairing symmetry in iron-based superconductors is based on weak-coupling BCS-like approaches²³⁻³⁸. It is believed that the Fe-As layers are responsible for the superconductivity and Ln-O layers provide electron carriers through fluorine doping, or very recently by simply introducing oxygen vacancies³⁹.

The theoretically calculated Fermi surface for '1111' system⁴⁰⁻⁴² consists of quasi-two-dimensional (2D) hole sheets centered at the P point and two electrons sheets at the M point of the first Brillouin zone. Within the so called minimal two-band model, these four bands considered as two effective 2D bands⁴³. Correspondingly, several of the available theoretical and experimental data clearly reveal that these materials are multi-band superconductors with s-type symmetry of the order parameter^{17,18}. Knight shift measurements in '1111' – class of Fe-As based compounds⁴³ have proven unambiguously the spin-singlet type pairing in these materials. Preliminary data by angle resolved photo-emission spectroscopy (ARPES) on crystals $\text{Ba}_{0.6}\text{K}_{0.4}\text{Fe}_2\text{As}_2$ have shown two groups of superconducting gaps ($\Delta_1 \approx 12$ meV, $\Delta_2 \approx 6$ meV) all with s-wave symmetry¹¹. Several data were reported in favour of S^\pm (Ref. 44) or S^{++} (Ref. 24), making the experimental situation about these compounds quite uncertain. The perception that the pairing mechanism may be triggered by anti-ferromagnetic fluctuations, similarly as in the cuprates, has motivated a considerable theoretical effort to understand the properties of multi-orbital Hubbard models and the dominant pairing mechanism upon doping^{17,45,46}.

The main anomaly of Fe As compounds is their multiple band nature. Electronic structure in a narrow enough energy interval around the Fermi level is formed almost only from the d-states of the iron. This

indicates that the lattice plays non-negligible role for superconductivity.

The theoretical study for a two band superconductor with very specific predications as to how the two gaps evolve with temperature, has been presented. Study of density of states and specific heat is also presented in the present paper.

2 Model Hamiltonian

The model Hamiltonian has the form⁴⁷ :

$$H = H_0^p + H_0^d + H_{pd} \quad \dots(1)$$

where

$$H_0^p = \sum_p \epsilon_p \left(C_{p\uparrow}^+ C_{p\uparrow} + C_{-p\downarrow}^+ C_{-p\downarrow} \right) + \Delta_{pp}^+ \sum_p C_{-p\downarrow} C_{p\uparrow} + \Delta_{pp} \sum_p C_{p\uparrow}^+ C_{-p\downarrow}^+ \quad \dots(2)$$

$$H_0^d = \sum_d \epsilon_d \left(C_{d\uparrow}^+ C_{d\uparrow} + C_{-d\downarrow}^+ C_{-d\downarrow} \right) + \Delta_{dd}^+ \sum_d C_{-d\downarrow} C_{d\uparrow} + \Delta_{dd} \sum_d C_{d\uparrow}^+ C_{-d\downarrow}^+ \quad \dots(3)$$

and

$$H_{pd} = V_{pd} \left\langle C_{p\uparrow}^+ C_{-p\downarrow}^+ \right\rangle \sum_d C_{-d\downarrow} C_{d\uparrow} + V_{pd} \left\langle C_{-d\downarrow} C_{d\uparrow} \right\rangle \sum_p C_{p\uparrow}^+ C_{-p\downarrow}^+ + V_{pd} \left\langle C_{d\uparrow}^+ C_{-d\downarrow}^+ \right\rangle \sum_p C_{-p\downarrow} C_{p\uparrow} + V_{pd} \left\langle C_{-p\downarrow} C_{p\uparrow} \right\rangle \sum_d C_{d\uparrow}^+ C_{-d\downarrow}^+ \quad \dots(4)$$

where p and d are momentum labels in the p and d bands respectively with energies ϵ_p and ϵ_d , μ is the common chemical potential. Each band has its proper pairing interaction V_{pp} and V_{dd} , while the pair interchange between the two bands is assured by V_{pd} term.

We have assumed $V_{pd} = V_{dp}$, and we define the following quantities:

$$\epsilon_p = \epsilon_p^0 - \mu \quad \epsilon_d = \epsilon_d^0 - \mu$$

$$\Delta_{pp}^+ = V_{pp} \left\langle C_{p\uparrow}^+ C_{-p\downarrow}^+ \right\rangle$$

$$\Delta_{dd}^+ = V_{dd} \left\langle C_{d\uparrow}^+ C_{-d\downarrow}^+ \right\rangle$$

Further, we define:

$$\begin{aligned}\Delta_1^+ &= V_{pd} \langle C_{p\uparrow}^+ C_{-p\downarrow}^+ \rangle \\ \Delta_2^+ &= V_{pd} \langle C_{d\uparrow}^+ C_{-d\downarrow}^+ \rangle\end{aligned}\quad \dots(5)$$

Now H_{pd} in Eq. (1) reads as :

$$\begin{aligned}H_{pd} &= \Delta_1^+ \sum_d C_{-d\downarrow} C_{d\uparrow} + \Delta_2^+ \sum_p C_{-p\downarrow}^+ C_{p\uparrow}^+ \\ &+ \Delta_2^+ \sum_p C_{-p\downarrow} C_{p\uparrow} + \Delta_1^+ \sum_d C_{d\uparrow}^+ C_{-d\downarrow}^+\end{aligned}$$

Final Hamiltonian can be written as:

$$\begin{aligned}H &= \sum_p \epsilon_p (C_{p\uparrow}^+ C_{p\uparrow} + C_{-p\downarrow}^+ C_{-p\downarrow}) \\ &+ \Delta_{pp}^+ \sum_p C_{-p\downarrow} C_{p\uparrow} + \Delta_{pp} \sum_p C_{p\uparrow}^+ C_{-p\downarrow}^+ \\ &+ \sum_d \epsilon_d (C_{d\uparrow}^+ C_{d\uparrow} + C_{-d\downarrow}^+ C_{-d\downarrow}) \\ &+ \Delta_{dd}^+ \sum_d C_{-d\downarrow} C_{d\uparrow} + \Delta_{dd} \sum_d C_{d\uparrow}^+ C_{-d\downarrow}^+ \\ &+ \Delta_1^+ \sum_d C_{-d\downarrow} C_{d\uparrow} + \Delta_2^+ \sum_p C_{-p\downarrow}^+ C_{p\uparrow}^+ \\ &+ \Delta_2^+ \sum_p C_{-p\downarrow} C_{p\uparrow} + \Delta_1^+ \sum_d C_{d\uparrow}^+ C_{-d\downarrow}^+\end{aligned}\quad \dots(6)$$

We study the Hamiltonian given in Eq. (6) with the Green's function technique and equation of motion method.

2.1 Green's Functions

In order to study the physical properties, we define the following normal and anomalous Green's functions⁴⁸⁻⁵⁸:

$$\begin{aligned}(a) \quad G_p(p, \tau - \tau') &= -\langle T_\tau C_{p\uparrow}(\tau) C_{p\uparrow}^+(\tau') \rangle \\ (b) \quad G_d(d, \tau - \tau') &= -\langle T_\tau C_{d\uparrow}(\tau) C_{d\uparrow}^+(\tau') \rangle \\ (c) \quad f_p(p, \tau - \tau') &= \langle T_\tau C_{-p\downarrow}(\tau) C_{p\uparrow}(\tau') \rangle \\ (d) \quad f_d(d, \tau - \tau') &= \langle T_\tau C_{-d\downarrow}(\tau) C_{d\uparrow}(\tau') \rangle \\ (e) \quad f_p^+(p, \tau - \tau') &= \langle T_\tau C_{p\uparrow}^+(\tau) C_{-p\downarrow}^+(\tau') \rangle \\ (f) \quad f_d^+(d, \tau - \tau') &= \langle T_\tau C_{d\uparrow}^+(\tau) C_{-d\downarrow}^+(\tau') \rangle\end{aligned}\quad \dots(7)$$

Following Green's functions technique and assuming, one obtains:

$$\begin{aligned}(\Delta_{pp} + \Delta_2) &= \bar{\Delta}_p \quad \text{and} \quad \Delta_{pp}^+ \cong \Delta_{pp} \\ (\Delta_{dd} + \Delta_1) &= \bar{\Delta}_d \quad \text{and} \quad \Delta_{dd}^+ \cong \Delta_{dd} \\ (\omega - \epsilon_p) \langle\langle C_{p\uparrow}, C_{p\uparrow}^+ \rangle\rangle &= 1 - \bar{\Delta}_p \langle\langle C_{p\uparrow}^+, C_{-p\downarrow}^+ \rangle\rangle\end{aligned}\quad \dots(8)$$

$$(\omega - \epsilon_d) \langle\langle C_{d\uparrow}, C_{d\uparrow}^+ \rangle\rangle = 1 - \bar{\Delta}_d \langle\langle C_{d\uparrow}^+, C_{-d\downarrow}^+ \rangle\rangle \quad \dots(9)$$

$$(\omega - \epsilon_p) \langle\langle C_{-p\downarrow}, C_{p\uparrow} \rangle\rangle = -\bar{\Delta}_p \langle\langle C_{p\uparrow}^+, C_{p\uparrow} \rangle\rangle \quad \dots(10)$$

$$(\omega - \epsilon_d) \langle\langle C_{-d\downarrow}, C_{d\uparrow} \rangle\rangle = -\bar{\Delta}_d \langle\langle C_{d\uparrow}^+, C_{d\uparrow} \rangle\rangle \quad \dots(11)$$

$$(\omega + \epsilon_p) \langle\langle C_{p\uparrow}^+, C_{-p\downarrow}^+ \rangle\rangle = -\bar{\Delta}_p \langle\langle C_{p\uparrow}, C_{p\uparrow} \rangle\rangle \quad \dots(12)$$

$$(\omega + \epsilon_d) \langle\langle C_{d\uparrow}^+, C_{-d\downarrow}^+ \rangle\rangle = -\bar{\Delta}_d \langle\langle C_{d\uparrow}, C_{d\uparrow} \rangle\rangle \quad \dots(13)$$

$$(\omega + \epsilon_p) \langle\langle C_{p\uparrow}^+, C_{p\uparrow} \rangle\rangle = 1 - \bar{\Delta}_p \langle\langle C_{-p\downarrow}, C_{p\uparrow} \rangle\rangle \quad \dots(14)$$

$$(\omega + \epsilon_d) \langle\langle C_{d\uparrow}^+, C_{d\uparrow} \rangle\rangle = 1 - \bar{\Delta}_d \langle\langle C_{-d\downarrow}, C_{d\uparrow} \rangle\rangle \quad \dots(15)$$

Finally, one obtains the Green's functions by solving coupled Eqs (8) to (15) as:

(a) Green's functions for p-band:

$$\langle\langle C_{p\uparrow}, C_{p\uparrow}^+ \rangle\rangle = \frac{(\omega + \epsilon_p)}{(\omega^2 - E_p^2)} \quad \dots(16)$$

$$\langle\langle C_{p\uparrow}^+, C_{-p\downarrow}^+ \rangle\rangle = -\frac{\bar{\Delta}_p}{(\omega^2 - E_p^2)} \quad \dots(17)$$

(b) Green's functions for d-band:

$$\langle\langle C_{d\uparrow}, C_{d\uparrow}^+ \rangle\rangle = \frac{(\omega + \epsilon_d)}{(\omega^2 - E_d^2)} \quad \dots(18)$$

$$\langle\langle C^+_{d\uparrow}, C^+_{-d\downarrow} \rangle\rangle = -\frac{\bar{\Delta}_d}{(\omega^2 - E_d^2)} \dots (19)$$

2.2 Correlation Functions

Using the following relation⁵²⁻⁵⁶:

$$\langle B(t') A(t) \rangle = \lim_{\epsilon \rightarrow 0} \frac{i}{2\pi} \int_{-\infty}^{+\infty} \frac{\langle\langle A(t') ; B(t') \rangle\rangle_{\omega+i\epsilon} - \langle\langle A(t') ; B(t') \rangle\rangle_{\omega-i\epsilon}}{e^{\beta\omega} + 1} \times \exp(-i\omega(t-t')) d\omega \dots(20)$$

and employing the following identity:

$$\lim_{\epsilon \rightarrow 0} \left(\frac{1}{\omega + i\epsilon - E_K} - \frac{1}{\omega - i\epsilon - E_K} \right) = 2\pi i \delta(\omega - E_K)$$

we obtain the correlation functions for the Green's functions given by Eqs (16) and (17) as:

$$\langle C^+_{p\uparrow} C_{p\uparrow} \rangle = f(\alpha_2) + \left[\frac{\alpha_1 - \epsilon_p}{(\alpha_1 - \alpha_2)} \right] [f(\alpha_1) - f(\alpha_2)] \dots(21)$$

$$\langle C^+_{p\uparrow} C^+_{-p\downarrow} \rangle = \frac{\bar{\Delta}_p}{(\alpha_1 - \alpha_2)} [f(\alpha_1) - f(\alpha_2)] \dots (22)$$

where

$$\alpha_1 = +\sqrt{\epsilon_p^2 + \Delta_{pp}^2 + \Delta_2^2 + \Delta_{pp}^+ \Delta_2 + \Delta_2^+ \Delta_{pp}} = +\sqrt{\epsilon_p^2 + (\Delta_{pp} + \Delta_2)^2} = +\sqrt{\epsilon_p^2 + \bar{\Delta}_p^2}$$

$$\alpha_2 = -\sqrt{\epsilon_p^2 + \Delta_{pp}^2 + \Delta_2^2 + \Delta_{pp}^+ \Delta_2 + \Delta_2^+ \Delta_{pp}} = -\sqrt{\epsilon_p^2 + (\Delta_{pp} + \Delta_2)^2} - \sqrt{\epsilon_p^2 + \bar{\Delta}_p^2} \dots(23)$$

and $f(\alpha_1)$ & $f(\alpha_2)$ are Fermi functions.

Similarly, correlation functions for Green's functions given in Eqs (18) and (19) for d band are obtained.

One can define the two superconducting order parameters related to the correlation functions corresponding to Green's functions $\langle\langle C^+_{p\uparrow}, C^+_{-p\downarrow} \rangle\rangle$ and $\langle\langle C^+_{d\uparrow}, C^+_{-d\downarrow} \rangle\rangle$ for p and d bands, respectively.

3 Physical Properties of Superconductors

3.1 Superconducting Order Parameters

Gap parameter $\bar{\Delta}$ is the superconducting order parameter, which can be determined self-consistently from the gap equation.

$$\bar{\Delta}_p = \Delta_{pp} + \Delta_2 \equiv V_{pp} f_p + V_{pd} f_d \dots(24)$$

$$\bar{\Delta}_d = \Delta_{dd} + \Delta_1 \equiv V_{pd} f_p + V_{dd} f_d \dots(25)$$

In a matrix form, the order parameter for the superconducting state is given⁴⁷ by :

$$\bar{\Delta}_i = \sum_j V_{ij} G(\bar{\Delta}_j) \bar{\Delta}_j \dots(26)$$

where $|V_{ij}|$ is the pairing interaction constant and function G's are defined as :

$$G(\bar{\Delta}_p) = N_p(0) \int_0^{\hbar\omega_p} \frac{d\epsilon_p}{E_p} \tanh \frac{E_p}{2k_B T} \dots (27)$$

$$G(\bar{\Delta}_d) = N_d(0) \int_0^{\hbar\omega_d} \frac{d\epsilon_d}{E_d} \tanh \frac{E_d}{2k_B T} \dots (28)$$

where $N_p(0)$ and $N_d(0)$ are density of states for p and d bands, respectively at the Fermi level.

We obtain two superconducting gaps corresponding to p and d bands in this interband model.

One can write the equations for superconducting gaps for p and d bands as follows:

$$\bar{\Delta}_p = V_{pd} G(\bar{\Delta}_d) \bar{\Delta}_d + V_{pp} G(\bar{\Delta}_p) \bar{\Delta}_p \dots(29)$$

$$\bar{\Delta}_d = V_{dp} G(\bar{\Delta}_p) \bar{\Delta}_p + V_{dd} G(\bar{\Delta}_d) \bar{\Delta}_d \quad \dots(30)$$

where V_{pp} and V_{dd} are pairing interaction for p and d bands, respectively, while the pair interchange between the two bands is assured by the V_{pd} term. The quantity V_{pd} has been supposed to be operative and constant in the energy interval for higher band and lower band, keeping in mind the integration ranges, the gap order parameter satisfies the system.

If the interband interactions are missing i.e. $V_{pp}=V_{dd}=0$, the transition is solely induced by the interband interaction⁴⁷ is :

$$k_B T_c = 1.14 \hbar \omega_c \exp \left[- \frac{1}{|V_{pd} \sqrt{N_p N_d}|} \right] \quad \dots(31)$$

One can easily show that by taking $V_{pp}=V_{dd}=0$, the result remains almost unaffected and interband interaction can induce the superconducting transition temperature T_c . Kristoffel *et al*⁵⁹. have shown that interband pairing is very efficient in enhancing T_c . This is a characteristic feature of interband models.

One can write the simultaneous equation as:

$$\frac{V_{pd} G(\bar{\Delta}_d)}{[1 - V_{pp} G(\bar{\Delta}_p)]} \times \frac{V_{pd} G(\bar{\Delta}_p)}{[1 - V_{pp} G(\bar{\Delta}_d)]} = 1 \quad \dots(32)$$

$$\bar{\Delta} = \bar{\Delta}_p + \bar{\Delta}_d = (V_{pd} + V_{pp}) (G(\bar{\Delta}_p) \bar{\Delta}_p + G(\bar{\Delta}_d) \bar{\Delta}_d) \quad \dots(33)$$

For the study of superconducting order parameter for $\text{Sm}_{0.95}\text{La}_{0.05}\text{O}_{0.85}\text{F}_{0.85}\text{Fe}_{0.15}\text{FeAs}$ ($T_c=57.3$ K) and $\text{SmO}_{1-x}\text{F}_x\text{FeAs}$ ($T_c=50$ K) systems with two band model, one finds following different situations: (i) The superconducting order parameters in the presence of p-band only and (ii) The superconducting order parameters in the presence of d-band only.

(a) SC order parameter for p and d bands

Using Eq. (41) with changes in variables as $\bar{\Delta}_p = x \times 10^{-21}$ J, $\epsilon_p = \hbar \omega_p y$, $d \in_p = \hbar \omega_p dy$, and taking $\mu=0$ in the absence of doping, after simplification, we obtain:

$$\begin{aligned} & V_{pd} N_d(0) \int_0^1 \frac{dy}{\sqrt{y^2 + 0.5797 x^2}} \\ & \times \left(\frac{1}{e^{\frac{-58}{T} \sqrt{y^2 + 0.5797 x^2}} + 1} - \frac{1}{e^{\frac{58}{T} \sqrt{y^2 + 0.5797 x^2}} + 1} \right) \\ & \left[1 - V_{pp} N_p(0) \int_0^1 \frac{dy}{\sqrt{y^2 + 0.4444 x^2}} \right. \\ & \times \left. \left(\frac{1}{e^{\frac{-108}{T} \sqrt{y^2 + 0.4444 x^2}} + 1} - \frac{1}{e^{\frac{108}{T} \sqrt{y^2 + 0.4444 x^2}} + 1} \right) \right] \\ & V_{pd} N_p(0) \int_0^1 \frac{dy}{\sqrt{y^2 + 0.4444 x^2}} \\ & \times \left(\frac{1}{e^{\frac{-108}{T} \sqrt{y^2 + 0.4444 x^2}} + 1} - \frac{1}{e^{\frac{108}{T} \sqrt{y^2 + 0.4444 x^2}} + 1} \right) = 1 \\ & \left[1 - V_{pd} N_d(0) \int_1^1 \frac{dy}{\sqrt{y^2 + 0.5797 x^2}} \right. \\ & \times \left. \left(\frac{1}{e^{\frac{-58}{T} \sqrt{y^2 + 0.5797 x^2}} + 1} - \frac{1}{e^{\frac{58}{T} \sqrt{y^2 + 0.5797 x^2}} + 1} \right) \right] \quad \dots(34) \end{aligned}$$

Solving Eq. (34) numerically using values of various parameters from Table 1, the variation of superconducting order parameter ($\bar{\Delta}$) with temperature for p and d-bands has been studied. The values obtained from Eq. (34) are presented in Table 2 and the variation of superconducting order parameter with temperature for $\text{Sm}_{0.95}\text{La}_{0.05}\text{O}_{0.85}\text{F}_{0.85}\text{Fe}_{0.15}\text{FeAs}$ ($T_c=57.3$ K) is shown in Fig. 1 and for system $\text{SmO}_{1-x}\text{F}_x\text{FeAs}$ ($T_c=50$ K) values are recorded in Table 3 and variation is shown in Fig. 2 for both p and d bands.

(b) SC order parameter in the presence of both p and d bands

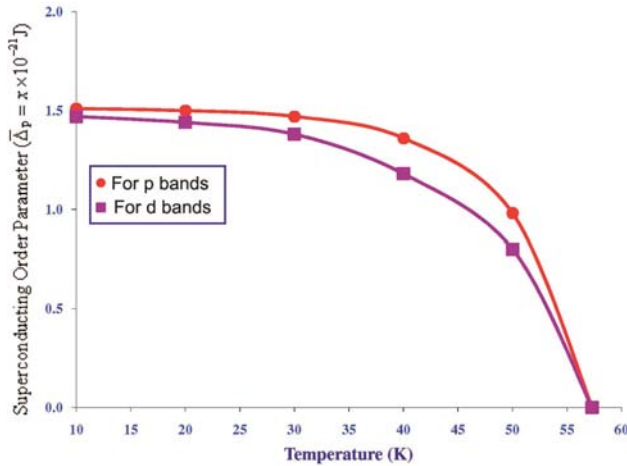
We have numerically depicted ($\bar{\Delta} = \bar{\Delta}_p + \bar{\Delta}_d$) with temperature for $\text{Sm}_{0.95}\text{La}_{0.05}\text{O}_{0.85}\text{F}_{0.85}\text{Fe}_{0.15}\text{FeAs}$ ($T_c=57.3$ K) in Table 2 and for system $\text{SmO}_{1-x}\text{F}_x\text{FeAs}$ ($T_c=50$ K) in Table 3 and variation is shown in Fig. 3.

Table 1 — Values of various parameters for $\text{Sm}_{0.95}\text{La}_{0.05}\text{O}_{0.85}\text{F}_{0.85}\text{Fe}_{0.15}\text{FeAs}$ ($T_c=57.3$ K) and $\text{SmO}_{1-x}\text{F}_x\text{FeAs}$ ($T_c=50$ K) (64)

S. No.	Parameter	Value	Reference
1	Phonon energy ($\hbar\omega_p$) for p band	$1.6 \times 10^{-21} \text{ J}$ $1.6 \times 10^{-21} \text{ J}$	[61]
2	Phonon energy ($\hbar\omega_p$) for d band	$1.5 \times 10^{-21} \text{ J}$	[61]
3	Density of states at the Fermi surface $N(0)$	$\cong 4.95 \times 10^{19} \text{ J/atom}$	[57]
4	Pairing interaction for p band (V_{pp})	$0.273 \times 10^{-19} \text{ J/atom}$	[62]
5	Pairing interaction for d band (V_{dd})	$0.280 \times 10^{-19} \text{ J/atom}$	[62]
6	The pair interchange between two bands (V_{pd})	1.75 eV	[63]
7	Density of states for d band $N_p(0)$	0.223 eV^{-1}	[63]
8	Density of states for p band $N_d(0)$	0.035 eV^{-1}	[63]
9	Number of atoms per unit volume	$\sim 4 \times 10^{22}$	[57,62]
10	Crystal Structure (1111 type)	ZrCuSiAs, type layered structure unit cell $a=b=0.3927 \text{ nm}$ and $c=0.8441 \text{ nm}$	[13]

Table 2 — Superconducting order parameter ($\bar{\Delta}_p$ & $\bar{\Delta}_d$) (p and d bands) for $\text{Sm}_{0.95}\text{La}_{0.05}\text{O}_{0.85}\text{F}_{0.85}\text{Fe}_{0.15}\text{FeAs}$ ($T_c=57.3$ K)

S.No.	Temperature (K)	$\bar{\Delta}_p = x \times 10^{-21} \text{ J}$	$\bar{\Delta}_d = x \times 10^{-21} \text{ J}$	$\bar{\Delta} = \bar{\Delta}_p + \bar{\Delta}_d$
1	10	1.51	1.47	2.98
2	20	1.50	1.44	2.94
3	30	1.47	1.38	2.85
4	40	1.36	1.18	2.54
5	50	0.98	0.80	1.78
6	57.3	0.00	0.00	0.00

Fig. 1 — Superconducting Order parameter for p and d bands ($\bar{\Delta}_p$ & $\bar{\Delta}_d$) for the system $\text{Sm}_{0.95}\text{La}_{0.05}\text{O}_{0.85}\text{F}_{0.85}\text{Fe}_{0.15}\text{FeAs}$ ($T_c=57.3$ K)

(c) $\frac{\bar{\Delta}_{p,d}(T)}{\bar{\Delta}_{p,d}(0)}$ with $\frac{T}{T_c}$: Variation of $\bar{\Delta}_p(T)/\bar{\Delta}_p(0)$

and $\bar{\Delta}_d(T)/\bar{\Delta}_d(0)$ with T/T_c is shown in Fig. 4 and corresponding values are given in Table 4.

(d) $\frac{2\bar{\Delta}_p}{kT_c}$ and $\frac{2\bar{\Delta}_d}{kT_c}$ with T: Variation of $2\bar{\Delta}_p/kT_c$ and $2\bar{\Delta}_d/kT_c$ with temperature (T) is shown in Fig. 5 and corresponding values are given in Table 5.

3.2 Electronic Specific Heat (C_{es})

The electronic specific heat per atom of a superconductor is determined from the following relation^{52-57,60},

(a) For p band

$$C_{es}^p = \frac{\partial}{\partial T} \frac{1}{N} \sum_p 2(\epsilon_p - \mu) \langle C_{p\uparrow}^+ C_{p\uparrow} \rangle \quad \dots(35)$$

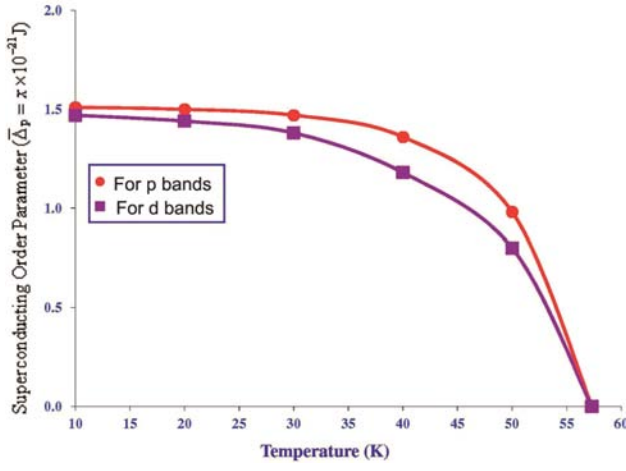
where ϵ_p is the energy of p band and μ is the common chemical potential.

Substituting $\langle C_{p\uparrow}^+ C_{p\uparrow} \rangle$ from Eq. (21) and changing the summation over p into an integration by using the relation $\sum_p = N(0) \int d\epsilon_p$

we obtain:

Table 3 — Superconducting order parameter ($\bar{\Delta}_p$ & $\bar{\Delta}_d$) (p and d bands) for $\text{SmO}_{1-x}\text{F}_x\text{FeAs}$ ($T_c=50$ K)

S.No.	Temperature (K)	$\bar{\Delta}_p = x \times 10^{-21}$ J	$\bar{\Delta}_d = x \times 10^{-21}$ J	$\bar{\Delta} = \bar{\Delta}_p + \bar{\Delta}_d$
1	10	1.76	1.74	3.50
2	20	1.72	1.70	3.42
3	30	1.58	1.54	3.12
4	40	1.27	1.15	2.42
5	50	0.00	0.00	0.00


 Fig. 2 — Superconducting Order parameter for p and d bands ($\bar{\Delta}_p$ & $\bar{\Delta}_d$) for the system $\text{SmO}_{1-x}\text{F}_x\text{FeAs}$ ($T_c=50$ K)

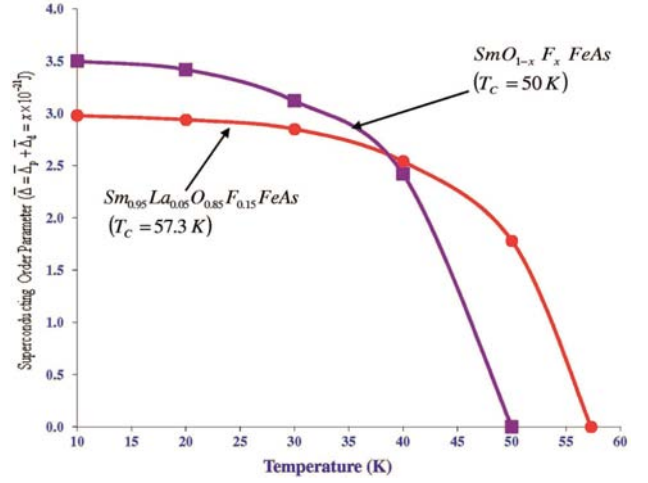
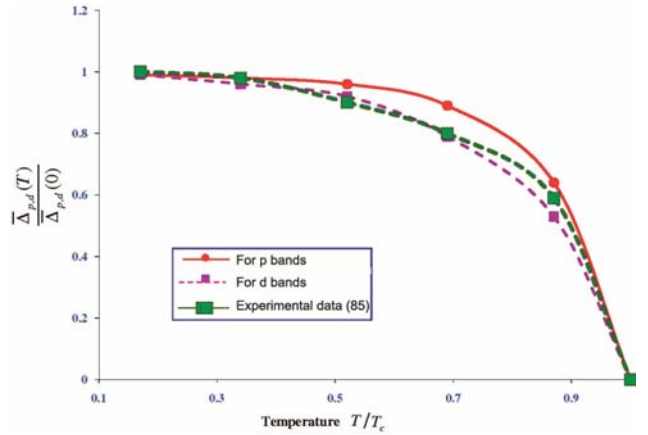
$$C_{es}^p = \frac{2N(0)}{N} \int_0^{\hbar\omega_p} d \left[\epsilon_p \frac{\beta \epsilon_p \alpha_2 \exp(\beta\alpha_2)}{T \{\exp(\beta\alpha_2) + 1\}^2} + \frac{\beta(\alpha_1 - \epsilon_p) \epsilon_p}{2T \sqrt{\epsilon_p^2 + \Delta_{pp}^2 + \Delta_2^2 + \Delta_{pp}^2 + \Delta_2^2 + \Delta_{pp}^2}} \times \left(\frac{\alpha_1 \exp(\beta\alpha_1)}{\{\exp(\beta\alpha_1) + 1\}^2} - \frac{\alpha_2 \exp(\beta\alpha_2)}{\{\exp(\beta\alpha_2) + 1\}^2} \right) \right] \quad \dots(36)$$

Where α_1 and α_2 are given by Eq. (23).

Using Eq. (36) and putting α_1 , α_2 and $\beta=1/kT$, after simplification, we obtain:

$$\frac{C_{es}^p}{T} = \frac{N(0)}{2NKT^3} \int_0^{\hbar\omega_p} d \epsilon_p \epsilon_p^2 \operatorname{sech}^2 \left(\frac{\sqrt{\epsilon_p^2 + \bar{\Delta}_p^2}}{2k_B T} \right) \quad \dots (37)$$

Using $\bar{\Delta}_p = x \times 10^{-21}$ J, $\epsilon_p = \hbar\omega_p y$, $d \epsilon_p = \hbar\omega_p dy$, and values of parameters from Table 1 with taking $\mu=0$ in the absence of doping, we obtain the


 Fig. 3 — Superconducting Order parameter ($\bar{\Delta}_p$ & $\bar{\Delta}_d$) for p and d bands for the systems $\text{Sm}_{0.95}\text{La}_{0.05}\text{O}_{0.85}\text{F}_{0.15}\text{FeAs}$ ($T_c=57.3$ K) and $\text{SmO}_{1-x}\text{F}_x\text{FeAs}$ ($T_c=50$ K)

 Fig. 4 — T/T_c versus $\frac{\bar{\Delta}_{p,d}(T)}{\bar{\Delta}_{p,d}(0)}$ for $\text{Sm}_{0.95}\text{La}_{0.05}\text{O}_{0.85}\text{F}_{0.15}\text{FeAs}$ ($T_c=57.3$ K)

expression for numerical study of specific heat for p-band as:

$$\frac{C_{es}^p}{T} = \frac{18.362 \times 10^{-44}}{T^3} \int_0^1 y^2 dy \operatorname{sech}^2 \left(\frac{36.23 \sqrt{2.56y^2 + x^2}}{T} \right) \quad \dots (38)$$

(b) For d band

Similarly, one obtains the expression for electronic specific heat C_{es}^d for d band as:

$$C_{es}^d = \frac{2N(0)}{N} \int_0^{\hbar\omega_d} d\epsilon_d \left[\frac{\beta \epsilon_d \alpha_2 \exp(\beta\alpha_2)}{T \{\exp(\beta\alpha_2) + 1\}^2} + \frac{\beta(\alpha_1 - \epsilon_d) \epsilon_d}{2T \sqrt{\epsilon_d^2 + \Delta_{dd}^2 + \Delta_1^2 + \Delta_{dd}^+ \Delta_1 + \Delta_1^+ \Delta_{dd}}} \times \left(\frac{\alpha_1 \exp(\beta\alpha_1)}{\{\exp(\beta\alpha_1) + 1\}^2} - \frac{\alpha_2 \exp(\beta\alpha_2)}{\{\exp(\beta\alpha_2) + 1\}^2} \right) \right] \dots(39)$$

In the absence of doping ($\mu=0$), we can study specific heat divided by T for d band numerically from the following expression:

Table 4 — $\frac{\bar{\Delta}_{p,d}(T)}{\bar{\Delta}_{p,d}(0)}$ versus T/T_c for $\text{Sm}_{0.95}\text{La}_{0.05}\text{O}_{0.85}\text{F}_{0.85}\text{Fe}_{0.15}\text{FeAs}$ ($T_c=57.3$ K)

S. No.	Temperature T/T_c	Theoretical		Experimental [65]
		For p band	For d band	
1	0.17	0.99	0.99	1.00
2	0.34	0.98	0.96	0.98
3	0.52	0.96	0.92	0.90
4	0.69	0.89	0.79	0.80
5	0.87	0.64	0.53	0.59
6	1.00	0.00	0.00	0.00

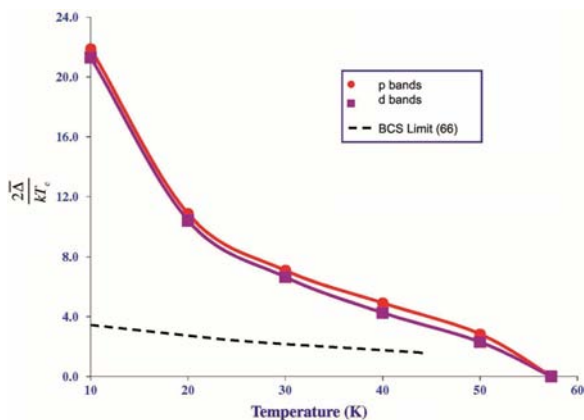


Fig. 5 — $\frac{2\bar{\Delta}_p}{kT_c}$ and $\frac{2\bar{\Delta}_d}{kT_c}$ versus T for $\text{Sm}_{0.95}\text{La}_{0.05}\text{O}_{0.85}\text{F}_{0.85}\text{Fe}_{0.15}\text{FeAs}$ ($T_c=57.3$ K)

$$\frac{C_{es}^d}{T} = \frac{15.131 \times 10^{-44}}{T^3} \int_0^1 y^2 dy \operatorname{sech}^2 \left(\frac{36.23 \sqrt{2.25y^2 + x^2}}{T} \right) \dots(40)$$

where α_1 and α_2 are similar to p band except the subscript p in Eq. (23) is replaced by d.

The values of electronic specific heat (C_{es}^p/T) versus T for $\text{Sm}_{0.95}\text{La}_{0.05}\text{O}_{0.85}\text{F}_{0.85}\text{Fe}_{0.15}\text{FeAs}$ ($T_c=57.3$ K) and $\text{SmO}_{1-x}\text{F}_x\text{FeAs}$ ($T_c=50$ K) systems for p band and d band are given in Tables 6 and 7 and variations are shown in Figs 6 and 7, respectively. A comparison with experimental results for $\text{SmO}_{1-x}\text{F}_x\text{FeAs}$ ($x=0.15$) superconductor is shown in Fig. 7. The agreement between theory and experiments is quite satisfactory.

3.3 Density of States N (ω)

The density of states is an important function. This helps in the interpretation of several experimental data, e.g. many processes that could occur in crystal but are forbidden because they do not conserve energy. Some of them nevertheless take place, provided to correct the energy imbalance by phonon-assisted processes, which are proportional⁵⁴ to

Table 5 — $\frac{2\bar{\Delta}_p}{kT_c}$ and $\frac{2\bar{\Delta}_d}{kT_c}$ versus T for p and d bands for $\text{Sm}_{0.95}\text{La}_{0.05}\text{O}_{0.85}\text{F}_{0.85}\text{Fe}_{0.15}\text{FeAs}$ ($T_c=57.3$ K)

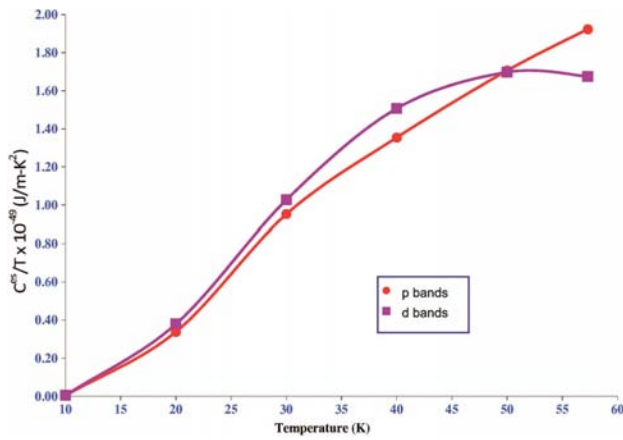
S. No.	Temperature (K)	$\frac{2\bar{\Delta}_p}{kT_c} = x \times 10^{-21}$	$\frac{2\bar{\Delta}_d}{kT_c} = x \times 10^{-21}$
1	10	21.88	21.30
2	20	10.86	10.43
3	30	7.10	6.66
4	40	4.92	4.27
5	50	2.84	2.31
6	57.3	0.00	0.00

Table 6 — Electronic specific heat with temperature (C_{es}^p & C_{es}^d p and d bands) for $\text{Sm}_{0.95}\text{La}_{0.05}\text{O}_{0.85}\text{F}_{0.85}\text{Fe}_{0.15}\text{FeAs}$ ($T_c=57.3$ K)

S. No.	Temperature (K)	$C_{es}^p/T \times 10^{-49}$ $J/m-k^2$ (For p band)	$C_{es}^d/T \times 10^{-49}$ $J/m-k^2$ (For d band)
1	10	0.0043	0.0055
2	20	0.3385	0.3810
3	30	0.9533	1.0280
4	40	1.3550	1.5080
5	50	1.7060	1.6980
6	57.3	1.9232	1.6755

Table 7 — Electronic specific heat with temperature $\left(\frac{C_{es}^p}{T} \& \frac{C_{es}^d}{T}\right)$ (p and d bands) for $\text{SmO}_{1-x}\text{F}_x\text{FeAs}$ ($T_c=50$ K)

S. No.	Temperature (K)	$C_{es}^p/T \times 10^{-49}$	$C_{es}^d/T \times 10^{-49}$	$C_{es}/T \times 10^{-49}$
		$J/m-k^2$ Theoretical	$J/m-k^2$ Theoretical	$J/m-k^2$ Experimental [64]
1	10	0.00086	0.00095	0.000
2	20	0.172	0.170	0.124
3	30	0.773	0.755	0.472
4	40	1.518	1.563	0.680
5	50	2.524	2.228	0.762


 Fig.6 — Electronic Specific heat (C_{es}^p/T and C_{es}^d/T) with temperature (p and d bands) for $\text{SmO}_{0.95}\text{La}_{0.05}\text{O}_{0.85}\text{F}_{0.85}\text{Fe}_{0.15}\text{FeAs}$ ($T_c=57.3$ K).

$N(\omega)/N(0)$. For $\omega > 0$, the density of states per atom^{55,56} $N(\omega)$ is defined as:

$$N_p(\omega) = \lim_{\epsilon \rightarrow 0} \frac{i}{2\pi N} \sum_p [G_{\uparrow\uparrow}(p, \omega + i\epsilon) - G_{\uparrow\uparrow}(p, \omega - i\epsilon)] \quad \dots(41)$$

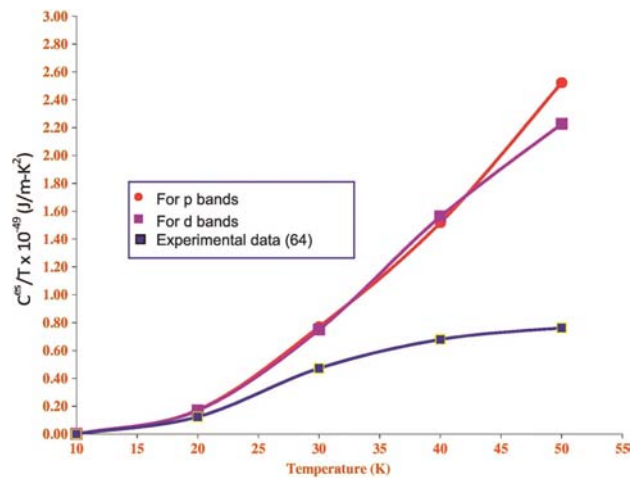
where $N_p(\omega)$ is the density of state function for p-band. For d-band, we have:

$$N_d(\omega) = \lim_{\epsilon \rightarrow 0} \frac{i}{2\pi N} \sum_d [G_{\uparrow\uparrow}(d, \omega + i\epsilon) - G_{\uparrow\uparrow}(d, \omega - i\epsilon)] \quad \dots(42)$$

Now substituting the Green function in Eq. (41) and using the delta function property, we obtain:

$$\lim_{\epsilon \rightarrow 0} \frac{i}{2\pi N} \left[\frac{1}{(\omega + i\epsilon - E_p)} - \frac{1}{(\omega - i\epsilon - E_p)} \right] = \delta(\omega - E_p)$$

We obtain,


 Fig.7 — Electronic Specific heat (C_{es}^p/T and C_{es}^d/T) with temperature (p and d bands) for $\text{SmO}_{1-x}\text{F}_x\text{FeAs}$ ($T_c=50$ K)

$$N_p(\omega) = \frac{1}{2} \sum_p \left[\left(1 + \frac{\epsilon_p}{E_p} \right) \delta(\omega - E_p) + \left(1 - \frac{\epsilon_p}{E_p} \right) \delta(\omega + E_p) \right] \quad \dots(43)$$

Changing the summation into integration with the help of following relation:

$$\sum_p = \int_{-h\omega_p}^{+h\omega_p} N_p(0) d\epsilon_p$$

where $N_p(0)$ is the density of states at absolute zero temperature, and further simplification of Eq. (43), yields

$$\frac{N_p(\omega)}{N_p(0)} = \begin{cases} 2 \frac{\omega}{\sqrt{\omega^2 - \bar{\Delta}_p^2}} & \text{for } \omega > 0 \\ 0 & \text{otherwise} \end{cases} \quad \dots(44)$$

Density of states function for the p band is given by Eq. (45). Now using the following values $\omega = y \times 10^{-21} J$, $\bar{\Delta}_p = x_1 \times 10^{-21} J$, $\bar{\Delta}_d = x_2 \times 10^{-21} J$, and taking $\mu = 0$ in the absence of doping, one obtains the expression for numerical study as :

$$\left(\frac{N_p(\omega)}{2N_p(0)} \right) = \frac{y \times 10^{-21}}{\sqrt{(y \times 10^{-21})^2 - (x_1 \times 10^{-21})^2}} \quad \dots (45)$$

Similarly, for d band, one can obtain the expression by replacing subscript p in Eq. (44) by d.

One obtains the expression for numerical study for d band, as:

Table 8 — Density of states with temperature for $\text{Sm}_{0.95}\text{La}_{0.05}\text{O}_{0.85}\text{F}_{0.85}\text{Fe}_{0.15}\text{FeAs}$ ($T_c=57.3$ K)

S No	$\omega = y \times 10^{-21} J$	$\frac{N(\omega)}{2N(0)}$	
		$\bar{\Delta}_p = 1.51 \times 10^{-21} J$ at T 10 K	$\bar{\Delta}_d = 1.47 \times 10^{-21} J$ at T 10 K
1	2	1.5250	1.4748
2	3	1.1573	1.1472
3	4	1.0799	1.0752
4	5	1.0490	1.0462
5	6	1.0333	1.0314
6	7	1.0241	1.0228
7	8	1.0183	1.0173
8	9	1.0144	1.0136
9	10	1.0116	1.0110
10	11	1.0096	1.0091
11	12	1.0080	1.0076
12	13	1.0068	1.0065

Table 9 — Density of states with temperature for $\text{SmO}_{1-x}\text{F}_x\text{FeAs}$ ($T_c=50$ K)

S No	$\omega = y \times 10^{-21} J$	$\frac{N(\omega)}{2N(0)}$	
		$\bar{\Delta}_p = 1.76 \times 10^{-21} J$ at T 10 K	$\bar{\Delta}_d = 1.74 \times 10^{-21} J$ at T 10 K
1	2	2.1054	2.0282
2	3	1.2348	1.2276
3	4	1.1136	1.1106
4	5	1.0684	1.0667
5	6	1.046	1.0449
6	7	1.0332	1.0324
7	8	1.0251	1.0245
8	9	1.0197	1.0192
9	10	1.0159	1.0155
10	11	1.0131	1.0128
11	12	1.0109	1.0107
12	13	1.0093	1.0091

$$\left(\frac{N_d(\omega)}{2N_d(0)} \right) = \frac{y \times 10^{-21}}{\sqrt{(y \times 10^{-21})^2 - (x_2 \times 10^{-21})^2}} \quad \dots(46)$$

The expressions given in Eqs (45) and (46) of density of states function for p and d band are similar, hence we have evaluated the values with different values of x for p and d bands.

The values of density of states from Eqs (45) and (46) for $\text{Sm}_{0.95}\text{La}_{0.05}\text{O}_{0.85}\text{F}_{0.85}\text{Fe}_{0.15}\text{FeAs}$ ($T_c=57.3$ K) and $\text{SmO}_{1-x}\text{F}_x\text{FeAs}$ ($T_c=50$ K) are given in Tables 8 and 9 and their respective behaviour are shown in Figs 8 and 9, respectively.

4 Results and Conclusions

In conclusion, we have described a two band model for the Fe-pnictides which we believe contains the essential physics of these materials. Following

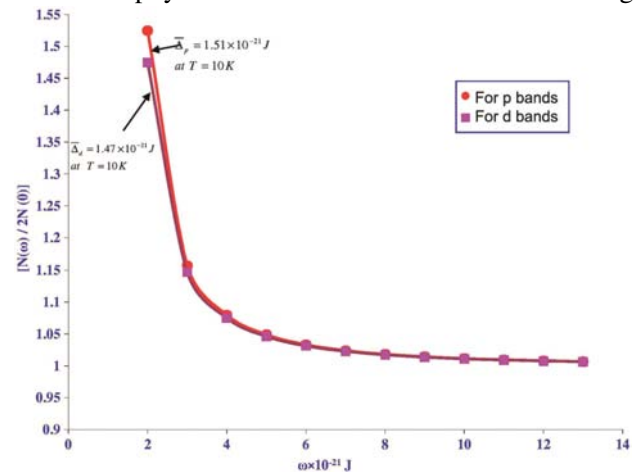


Fig. 8 — Density of states for $\text{Sm}_{0.95}\text{La}_{0.05}\text{O}_{0.85}\text{F}_{0.85}\text{Fe}_{0.15}\text{FeAs}$ ($T_c=57.3$ K)

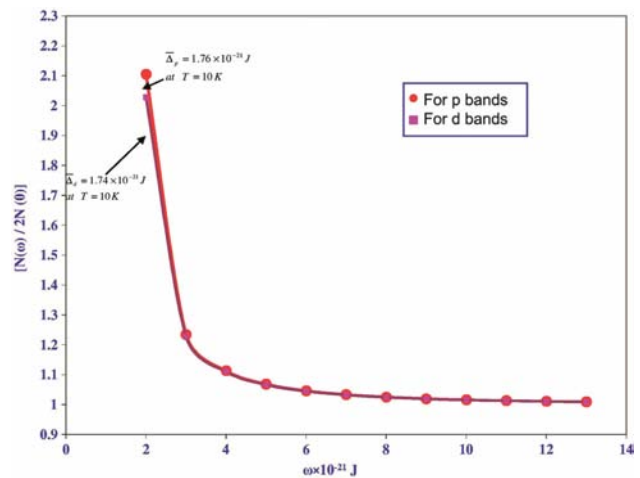


Fig. 9 — Density of states for $\text{SmO}_{1-x}\text{F}_x\text{FeAs}$ ($T_c=50$ K)

Green's functions technique and equation of motion method, we have obtained the expressions for superconducting order parameter ($\bar{\Delta}$), density of states, specific heat, for both p and d bands. Making use of values of various parameters given in Table 1 for the systems $\text{Sm}_{0.95}\text{La}_{0.05}\text{O}_{0.85}\text{F}_{0.85}\text{Fe}_{0.15}\text{FeAs}$ ($T_c=57.3$ K) (Ref. 8) and $\text{SmO}_{1-x}\text{F}_x\text{FeAs}$ ($T_c=50$ K) (Ref. 64), we have solved numerically the expressions given in Eq. (46) and wherever possible, compared our results with the available experimental data. We found:

- (i) The superconducting transition temperature (T_c) for $\text{Sm}_{0.95}\text{La}_{0.05}\text{O}_{0.85}\text{F}_{0.85}\text{Fe}_{0.15}\text{FeAs}$ is 57.3 K (Ref. 8) and for $\text{SmO}_{1-x}\text{F}_x\text{FeAs}$ is 50 K (Ref. 64) agrees well with experimental data.
- (ii) The variation of $\bar{\Delta} = \bar{\Delta}_p + \bar{\Delta}_d$ with temperature T for the system $\text{Sm}_{0.95}\text{La}_{0.05}\text{O}_{0.85}\text{F}_{0.85}\text{Fe}_{0.15}\text{FeAs}$ is found to be in good agreement with experimental data.
- (iii) The calculated values of $\frac{\bar{\Delta}_{p,d}(T)}{\bar{\Delta}_{p,d}(0)}$ versus T/T_c , $\frac{2\bar{\Delta}_p}{kT_c}$ and $\frac{2\bar{\Delta}_d}{kT_c}$ versus temperature T for p and d bands exhibit good agreement with experimental data for $\text{Sm}_{0.95}\text{La}_{0.05}\text{O}_{0.85}\text{F}_{0.85}\text{Fe}_{0.15}\text{FeAs}$ (Ref. 8)
- (iv) The behaviour of C_{es}/T versus T obtained from our model is in reasonable agreement with the experimental data for the system⁶⁴ $\text{SmO}_{1-x}\text{F}_x\text{FeAs}$.
- (v) Density of states study clearly supports the BCS-like coupling in these systems. Our results for density of states are intended to provide a basis for experimental comparisons.

The investigations reported here aim to establish several of the properties of two band model. Only a detailed comparison with experiments will clarify whether this simple model is or not a good approximation to describe the Fe-pnictides superconductors

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