Two- gap Superconductivity and Electronic Specific Heat in Binary Intermetallic Compound MgB_2 based with Intra-and Interband interactions

Pradeep Chaudhary
Department of Physics, Govt. Polytechnic College Chittorgarh 312001,Rajasthan, India.
E-mail-pchaudhary45@gmail.com

Anuj Nuwal*
Department of Physics, Swami Vivekanand Govt. Model school Mandal, Bhilwara 311403, Rajasthan, India.
E-mail- anuj.nuwal2011@gmail.com

S. C. Tiwari
Department of Physics, M.L.V. Govt. College Bhilwara 311001, Rajasthan, India.
E-mail- sct_123@rediff.com

*** Corresponding Author**

ABSTRACT

Magnesium diboride (MgB_2) with $T_C \approx 39K$ is a record breaking two gap superconducting compound among the s-p metals and alloys. Considering a multiband model Hamiltonian with intra- & inter band pair transfer interactions and following Green's function technique and equation of motion method, we have shown that MgB_2 possess two gaps and study of electronic specific heat. The agreement between theoretical results obtained and experimental results is quite convincing.

Keywords: Green's function, Superconducting order parameter, Electronic specific heat.
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1. Introduction:

The serendipitous discovery of superconductivity at 39K in the binary intermetallic MgB_2 by Nagamutsu et al. [1] has attracted great interest [2-7] and revived the multiband formalism proposed by Morton and Richard [8]. Experimental investigations have established presence of manifestations of two superconducting gaps in various response functions [4, 7]. Characteristic gap- to - T_C ratios violating the BCS universality have been found [4, 5]. These findings indicate to that simple one-band approach to MgB_2 must be generalized.

At the same time band structure calculations of MgB_2 [6,7] have shown various bands intersecting the Fermi level. Correspondingly a contribution of interband and intraband interactions in the pairing mechanism is expected [9-15]. The finding of central importance has been that various electron bands intersect the Fermi Level. The part of the spectrum which is effective for the superconductivity incorporates two pairs of bands. These are of boron $p_{x,y}$ and p_z origin (two B-planes) with two-dimensional σ- bonding and three- dimensional π bonding respectively. Number of experimental investigations using various techniques have revealed the quasi two gaps, $\Delta_\sigma = 7\ mev$ and $\Delta_\pi = 2.8\ mev$ due to σ and π type electron respectively [17-18].

The observation of two energy gaps and the considerable superconductive anisotropy as large as 6-9 [17-19] and called for a more thorough investigation in terms of two-band model with intra- and inter- band coupling.

In the present work a systematic study of two-band superconductivity model with intra- and interband pairing channels from first principles is developed and applied to MgB_2.We present the formalism in Section 2; Section 3 is devoted to physical properties as electronic specific heat; Section 4 is devoted to results while in Section 5 we present conclusions.

2 Theoretical formalism

The two band model Hamiltonian with intra & inter-band pair transfer interaction for our system has the form [20]

$$H = \sum_{\alpha l s} \in_\alpha (l) a^+_{\alpha l s} a_{\alpha l s} - \frac{1}{V} \sum_{\alpha\alpha'} \sum_{lm} W_{\alpha\alpha'}(l,m) a^+_{\alpha l\uparrow} a^+_{\alpha - l\downarrow} a_{\alpha' - m\downarrow} a_{\alpha' m\uparrow} \quad (1)$$

Where $\overline{\in}_\alpha = \in_\alpha - \mu$ is the electron energy in the bands α = 1, 2; μ is chemical potential; V is the volume of superconductor & $W_{\alpha\alpha'}(l, m)$ are the matrix elements of intra band interaction for α = α' and interband interaction for α≠α'.

We can write final Hamiltonian as –

$$H = H_{11} + H_{22} + H_{12} + H_{21} \quad (2)$$

Here

$$H_{11} = \sum_{ls} \overline{\in}_1 (l) a^+_{1ls} a_{1ls} - \frac{1}{V} \sum_{lm} W_{11}(l,m) a^+_{1l\uparrow} a^+_{1-l\downarrow} a_{1-m\downarrow} a_{1m\uparrow}$$

$$H_{22} = \sum_{ls} \overline{\in}_2 (l) a^+_{2ls} a_{2ls} - \frac{1}{V} \sum_{lm} W_{22}(l,m) a^+_{2l\uparrow} a^+_{2-l\downarrow} a_{2-m\downarrow} a_{2m\uparrow}$$

$$H_{12} = \sum_{ls} \overline{\in}_1 (l) a^+_{1ls} a_{1ls} - \frac{1}{V} \sum_{lm} W_{12}(l,m) a^+_{1l\uparrow} a^+_{1-l\downarrow} a_{2-m\downarrow} a_{2m\uparrow}$$

$$H_{21} = \sum_{ls} \overline{\in}_2 (l) a^+_{2ls} a_{2ls} - \frac{1}{V} \sum_{lm} W_{21}(l,m) a^+_{2l\uparrow} a^+_{2-l\downarrow} a_{1-m\downarrow} a_{1m\uparrow}$$

Thus

$$\begin{aligned} H = & \sum_{ls} \overline{\in}_1 (l) a^+_{1ls} a_{1ls} - \frac{1}{V} \sum_{lm} W_{11}(l,m) a^+_{1l\uparrow} a^+_{1-l\downarrow} a_{1-m\downarrow} a_{1m\uparrow} \\ & + \sum_{ls} \overline{\in}_2 (l) a^+_{2ls} a_{2ls} - \frac{1}{V} \sum_{lm} W_{22}(l,m) a^+_{2l\uparrow} a^+_{2-l\downarrow} a_{2-m\downarrow} a_{2m\uparrow} \\ & + \sum_{ls} \overline{\in}_1 (l) a^+_{1ls} a_{1ls} - \frac{1}{V} \sum_{lm} W_{12}(l,m) a^+_{1l\uparrow} a^+_{1-l\downarrow} a_{2-m\downarrow} a_{2m\uparrow} \\ & + \sum_{ls} \overline{\in}_2 (l) a^+_{2ls} a_{2ls} - \frac{1}{V} \sum_{lm} W_{21}(l,m) a^+_{2l\uparrow} a^+_{2-l\downarrow} a_{1-m\downarrow} a_{1m\uparrow} \end{aligned} \quad (3)$$

We have solved the above Hamiltonian with the help of Green's functions technique and equation of motion method [21-26].

2.1 Green's functions:

In order to study the physical properties of intermetallic binary superconductors, we define the following Green's functions for the model-

(a) $G_{11}(1, k, \uparrow) = \langle\langle a_{1k\uparrow} \mid a^{+}_{1k\uparrow} \rangle\rangle$

(b) $G_{22}(2, k, \uparrow) = \langle\langle a_{2k\uparrow} \mid a^{+}_{2k\uparrow} \rangle\rangle$

(c) $G_{21}(2, 1, k, \uparrow) = \langle\langle a_{2k\uparrow} \mid a^{+}_{1k\uparrow} \rangle\rangle$

(d) $G_{12}(1, 2, k, \uparrow) = \langle\langle a_{1k\uparrow} \mid a^{+}_{2k\uparrow} \rangle\rangle$

(e) $F_{11}(1, k, \uparrow) = \langle\langle a^{+}_{1-k\downarrow} \mid a^{+}_{1k\uparrow} \rangle\rangle$

(f) $F_{22}(2, k, \uparrow) = \langle\langle a^{+}_{2-k\downarrow} \mid a^{+}_{2k\uparrow} \rangle\rangle$

(g) $F_{21}(2, 1, k, \uparrow) = \langle\langle a^{+}_{2-k\downarrow} \mid a^{+}_{1k\uparrow} \rangle\rangle$

(h) $F_{12}(1, 2, k, \uparrow) = \langle\langle a^{+}_{1-k\downarrow} \mid a^{+}_{2k\uparrow} \rangle\rangle$ (4)

In this set of eight Green's functions, the first four are normal & last four are anomalous Green's functions [27-28].The time and temperature dependent Green's functions are quite suitable to study various physical properties of MgB_2.

Using the model Hamiltonian, one obtains the following equations of motion of Green's functions:

$$\omega_1^- G_{11} + W_{12}\gamma_{12}G_{21} + (W_{11}\Delta_{11} + W_{12}\Delta_{22})F_{11} + 0.F_{21} = 1 \quad (5)$$

$$\omega_2^- G_{22} + W_{12}\gamma_{21}G_{12} + (W_{12}\Delta_{11} + W_{22}\Delta_{22})F_{22} + 0.F_{12} = 1 \quad (6)$$

$$\omega_2^- G_{21} + W_{12}\gamma_{12}G_{11} + (W_{12}\Delta_{11} + W_{22}\Delta_{22})F_{21} + 0.F_{11} = 0 \quad (7)$$

$$\omega_1^- G_{12} + W_{12}\gamma_{12}G_{22} + (W_{11}\Delta_{11} + W_{12}\Delta_{22})F_{12} + 0.F_{22} = 0 \quad (8)$$

$$\omega_1^+ F_{11} - W_{21}\gamma_{21}F_{21} + (W_{11}\Delta^{+}_{11} + W_{21}\Delta^{+}_{22})G_{11} + 0.G_{21} = 0 \quad (9)$$

$$\omega_2^+ F_{22} - W_{12}\gamma_{12}F_{12} + (W_{12}\Delta^{+}_{11} + W_{22}\Delta^{+}_{22})G_{22} + 0.G_{12} = 0 \quad (10)$$

$$\omega_2^+ F_{21} - W_{12}\gamma_{12}F_{11} + (W_{12}\Delta^{+}_{11} + W_{22}\Delta^{+}_{22})G_{21} + 0.G_{11} = 0 \quad (11)$$

$$\omega_1^{+} F_{12} - W_{21}\gamma_{21} F_{22} + \left(W_{11}\Delta_{11}^{+} + W_{21}\Delta_{22}^{+}\right) G_{12} + 0.G_{22} = 0 \quad (12)$$

Where $\omega_1^{\pm} = \omega \pm \tilde{\in}_1 (k)$

& $\omega_2^{\pm} = \omega \pm \tilde{\in}_2 (k)$

We have used to the following notations

$$\tilde{\in}_1 (k) = \in_1 (k) - W_{11} n_{1-k\downarrow} \; \& \; \tilde{\in}_2 (k) = \in_2 (k) - W_{22} n_{2-k\downarrow}$$

$$n_{1-k\downarrow} = \frac{1}{V} < a_{1-k\downarrow}^{+} a_{1-k\downarrow} > \& \; n_{2-k\downarrow} = \frac{1}{V} < a_{2-k\downarrow}^{+} a_{2-k\downarrow} >$$

$$\gamma_{21} = \frac{1}{V} < a_{2-k\downarrow}^{+} a_{1-k\downarrow} > \& \; \gamma_{12} = \frac{1}{V} < a_{1-k\downarrow}^{+} a_{2-k\downarrow} >$$

$$\Delta_{11} = \frac{1}{V} < a_{1-k\downarrow} a_{1k\uparrow} > \& \; \Delta_{22} = \frac{1}{V} < a_{2-k\downarrow} a_{2k\uparrow} >$$

$$\Delta_{11}^{+} = \frac{1}{V} < a_{1k\uparrow}^{+} a_{1-k\downarrow}^{+} >> \& \; \Delta_{22}^{+} = \frac{1}{V} < a_{2k\uparrow}^{+} a_{2-k\downarrow}^{+} >>$$

To solve the above equations we have assumed:

$$\gamma_{21} = \gamma_{12} = \gamma$$

$$\Delta_{11} = \Delta_{11}^{+} = \Delta_1 \;\; \& \; \Delta_{22} = \Delta_{22}^{+} = \Delta_2$$

$$n_{1-k\downarrow} = n_{1k\uparrow} \; \& \; n_{2-k\downarrow} = n_{2k\uparrow}$$

$W_{11} = W_{22}$ & $W_{12} = W_{21}$

Now, we have two sets of equations. The first set includes equations (5), (7), (9) & (11)

as follows :

$$\omega_1^{-} G_{11} + W_{12}\gamma \, G_{21} + \left(W_{11}\Delta_1 + W_{12}\Delta_2\right) F_{11} + 0.F_{21} = 1$$

$$W_{12}\gamma \, G_{11} + \omega_2^{-} G_{21} + 0.F_{11} + \left(W_{12}\Delta_1 + W_{11}\Delta_2\right) F_{21} = 0$$

$$\left(W_{11}\Delta_1 + W_{12}\Delta_2\right) G_{11} + 0.G_{21} + \omega_1^{+} F_{11} - W_{12}\gamma \, F_{21} = 0$$

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$$0.G_{11} + (W_{12}\Delta_1 + W_{11}\Delta_2)G_{21} - W_{12}\gamma\, F_{11} + \omega_2^{+} F_{21} = 0$$

One obtains the Green's functions by solving above coupled equations

$$G_{11} = \frac{1}{2}\left[\frac{1}{\omega-\alpha_1} + \frac{1}{\omega+\alpha_1}\right] + \frac{\left[\tilde{\in}_1\left(\alpha_1^2-\alpha_2^2\right) + W_{12}^2\gamma^2(\tilde{\in}_1 + \tilde{\in}_2)\right]}{2\alpha_1\left(\alpha_1^2-\alpha_2^2\right)}.$$

$$\left[\frac{1}{\omega-\alpha_1} - \frac{1}{\omega+\alpha_1}\right] - \frac{W_{12}^2\gamma^2(\tilde{\in}_1 + \tilde{\in}_2)}{2\alpha_2\left(\alpha_1^2-\alpha_2^2\right)}\left[\frac{1}{\omega-\alpha_2} - \frac{1}{\omega+\alpha_2}\right] \tag{13}$$

$$G_{21} = \frac{W_{12}\gamma\left(\alpha_1^2 - P_2\right)}{2\alpha_1\left(\alpha_1^2-\alpha_2^2\right)}\left[-\frac{1}{\omega-\alpha_1} + \frac{1}{\omega+\alpha_1}\right] - \frac{W_{12}\gamma\left(\alpha_2^2 - P_2\right)}{2\alpha_2\left(\alpha_1^2-\alpha_2^2\right)}\left[-\frac{1}{\omega-\alpha_2} + \frac{1}{\omega+\alpha_2}\right]$$

$$+\frac{W_{12}\gamma(\tilde{\in}_1 + \tilde{\in}_2)}{2\left(\alpha_1^2-\alpha_2^2\right)}\left[\left(\frac{1}{\omega-\alpha_2} + \frac{1}{\omega+\alpha_2}\right) - \left(\frac{1}{\omega-\alpha_1} + \frac{1}{\omega+\alpha_1}\right)\right] \tag{14}$$

$$F_{11} = \frac{(W_{11}\Delta_1 + W_{12}\Delta_2)}{2\alpha_1}\left[-\frac{1}{\omega-\alpha_1} + \frac{1}{\omega+\alpha_1}\right]$$

$$+\frac{W_{12}^2\gamma^2\{(W_{11}\Delta_1 + W_{12}\Delta_2) - (W_{12}\Delta_1 + W_{11}\Delta_2)\}}{2\alpha_1\left(\alpha_1^2-\alpha_2^2\right)}\left[-\frac{1}{\omega-\alpha_1} + \frac{1}{\omega+\alpha_1}\right]$$

$$+\frac{W_{12}^2\gamma^2\{(W_{11}\Delta_1 + W_{12}\Delta_2) - (W_{12}\Delta_1 + W_{11}\Delta_2)\}}{2\alpha_2\left(\alpha_1^2-\alpha_2^2\right)}\left[\frac{1}{\omega-\alpha_2} - \frac{1}{\omega+\alpha_2}\right] \tag{15}$$

$$F_{21} = \frac{W_{12}\gamma}{2\left(\alpha_1^2-\alpha_2^2\right)}\{(W_{11}\Delta_1 + W_{12}\Delta_2) - (W_{12}\Delta_1 + W_{11}\Delta_2)\}$$

$$\left[-\left\{\frac{1}{\omega-\alpha_1} + \frac{1}{\omega+\alpha_1}\right\} + \left\{\frac{1}{\omega-\alpha_2} + \frac{1}{\omega+\alpha_2}\right\}\right]$$

$$+\frac{W_{12}\gamma}{2\alpha_1\left(\alpha_1^2-\alpha_2^2\right)}\{\tilde{\in}_2(W_{11}\Delta_1 + W_{12}\Delta_2) + \tilde{\in}_1(W_{12}\Delta_1 + W_{11}\Delta_2)\}.\left[\frac{1}{\omega-\alpha_1} - \frac{1}{\omega+\alpha_1}\right]$$

$$+\frac{W_{12}\gamma}{2\alpha_2\left(\alpha_1^2-\alpha_2^2\right)}\{\tilde{\in}_2(W_{11}\Delta_1 + W_{12}\Delta_2) + \tilde{\in}_1(W_{12}\Delta_1 + W_{11}\Delta_2)\}.\left[-\frac{1}{\omega-\alpha_2} + \frac{1}{\omega+\alpha_2}\right]$$

(16)

Where $\alpha_1^2 = \tilde{\in}_1^2 + (W_{11}\Delta_1 + W_{12}\Delta_2)^2 + W_{12}^2\gamma^2$

$\alpha_2^2 = \tilde{\in}_2^2 + (W_{12}\Delta_1 + W_{11}\Delta_2)^2 + W_{12}^2\gamma^2$

$$P_2 = (W_{11}\Delta_1 + W_{12}\Delta_2)(W_{12}\Delta_1 + W_{11}\Delta_2) + W_{12}^2\gamma^2 - \tilde{\in}_1\tilde{\in}_2 \tag{17}$$

The second set includes equations (6), (8), (10) & (12) as follows:

$$\omega_2^- G_{22} + W_{12}\gamma\, G_{12} + (W_{12}\Delta_1 + W_{11}\Delta_2)F_{22} + 0.F_{12} = 1$$

$$W_{12}\gamma\, G_{22} + \omega_1^- G_{12} + 0.F_{22} + (W_{11}\Delta_1 + W_{12}\Delta_2)F_{12} = 0$$

$$(W_{12}\Delta_1 + W_{11}\Delta_2)G_{22} + 0.G_{12} + \omega_2^+ F_{22} - W_{12}\gamma\, F_{12} = 0$$

$$0.G_{22} + (W_{11}\Delta_1 + W_{12}\Delta_2)G_{12} - W_{12}\gamma\, F_{22} + \omega_1^+ F_{12} = 0$$

We obtain following Green's functions by solving above coupled equations

$$G_{22} = \frac{1}{2}\left[\frac{1}{\omega-\alpha_2} + \frac{1}{\omega+\alpha_2}\right] + \frac{W_{12}^2\gamma^2(\tilde{\in}_1 + \tilde{\in}_2)}{2\alpha_1(\alpha_1^2-\alpha_2^2)}\left[\frac{1}{\omega-\alpha_1} - \frac{1}{\omega+\alpha_1}\right]$$
$$- \frac{\left\{\tilde{\in}_2\,(\alpha_2^2-\alpha_1^2) + W_{12}^2\gamma^2(\tilde{\in}_1+\tilde{\in}_2)\right\}}{2\alpha_2(\alpha_1^2-\alpha_2^2)}\left[\frac{1}{\omega-\alpha_2} - \frac{1}{\omega+\alpha_2}\right] \tag{18}$$

$$G_{12} = \frac{W_{12}\gamma(\alpha_1^2 - P_2)}{2\alpha_1(\alpha_1^2-\alpha_2^2)}\left[-\frac{1}{\omega-\alpha_1} + \frac{1}{\omega+\alpha_1}\right] - \frac{W_{12}\gamma(\alpha_2^2 - P_2)}{2\alpha_2(\alpha_1^2-\alpha_2^2)}\left[-\frac{1}{\omega-\alpha_2} + \frac{1}{\omega+\alpha_2}\right]$$
$$+ \frac{W_{12}\gamma(\tilde{\in}_1 + \tilde{\in}_2)}{2(\alpha_1^2-\alpha_2^2)}\left[\left\{\frac{1}{\omega-\alpha_2} + \frac{1}{\omega+\alpha_2}\right\} - \left\{\frac{1}{\omega-\alpha_1} + \frac{1}{\omega+\alpha_1}\right\}\right] \tag{19}$$

$$F_{22} = \frac{(W_{12}\Delta_1 + W_{11}\Delta_2)}{2\alpha_2}\left[-\frac{1}{\omega-\alpha_2} + \frac{1}{\omega+\alpha_2}\right]$$
$$+ \frac{W_{12}^2\gamma^2\left[(W_{12}\Delta_1 + W_{11}\Delta_2) - (W_{11}\Delta_1 + W_{12}\Delta_2)\right]}{2\alpha_1(\alpha_1^2-\alpha_2^2)}\left[-\frac{1}{\omega-\alpha_1} + \frac{1}{\omega+\alpha_1}\right]$$
$$+ \frac{W_{12}^2\gamma^2\left[(W_{12}\Delta_1 + W_{11}\Delta_2) - (W_{11}\Delta_1 + W_{12}\Delta_2)\right]}{2\alpha_2(\alpha_1^2-\alpha_2^2)}\left[\frac{1}{\omega-\alpha_2} - \frac{1}{\omega+\alpha_2}\right] \tag{20}$$

$$F_{12} = \frac{W_{12}\gamma}{2(\alpha_1^2 - \alpha_2^2)}\{(W_{12}\Delta_1 + W_{11}\Delta_2) - (W_{11}\Delta_1 + W_{12}\Delta_2)\}\left[\left(\frac{1}{\omega-\alpha_2} + \frac{1}{\omega+\alpha_2}\right) - \left(\frac{1}{\omega-\alpha_1} + \frac{1}{\omega+\alpha_1}\right)\right]$$

$$+ \frac{W_{12}\gamma}{2\alpha_1(\alpha_1^2 - \alpha_2^2)}\{\tilde{\in}_1 (W_{12}\Delta_1 + W_{11}\Delta_2) + \tilde{\in}_2 (W_{11}\Delta_1 + W_{12}\Delta_2)\}\left(\frac{1}{\omega-\alpha_1} - \frac{1}{\omega+\alpha_1}\right)$$

$$+ \frac{W_{12}\gamma}{2\alpha_2(\alpha_1^2 - \alpha_2^2)}\{\tilde{\in}_1 (W_{12}\Delta_1 + W_{11}\Delta_2) + \tilde{\in}_2 (W_{11}\Delta_1 + W_{12}\Delta_2)\}\left(-\frac{1}{\omega-\alpha_2} + \frac{1}{\omega+\alpha_2}\right)$$

(21)

2.2 Correlation Functions:

The various physical properties of the intermetallic binary system can be studied with the help of correlation functions of Green's functions (Eqs.13-21) [21-29]

To derive correlation functions we use the following relation

$$< B(t')A(t) >= \lim_{\in \to 0} \frac{i}{2\pi}\int_{-\infty}^{+\infty}\left[\frac{<< A(t');B(t) >>_{w+i\in} - << A(t');B(t) >>_{w-i\in}}{e^{\beta\omega}+1}\right]e^{-iw(t-t')}d\omega$$

and employing the following identity

$$\lim_{\in\to 0}\left(\frac{1}{\omega + i\in - E_k} - \frac{1}{\omega - i\in - E_k}\right) = 2\pi\, i\delta(\omega - E_K) \quad (22)$$

We obtain correlation functions for various Green's functions as 100

$$< a_{1-k\downarrow}a_{1k\uparrow} > = \frac{(W_{11}\Delta_1 + W_{12}\Delta_2)\tanh\frac{1}{2k_BT}\sqrt{\tilde{\in}_1^2 + (W_{11}\Delta_1 + W_{12}\Delta_2)^2 + W_{12}^2\gamma^2}}{2\sqrt{\tilde{\in}_1^2 + (W_{11}\Delta_1 + W_{12}\Delta_2)^2 + W_{12}^2\gamma^2}}$$

$$+ \frac{W_{12}^2\gamma^2 (W_{11}\Delta_1 + W_{12}\Delta_2 - W_{12}\Delta_1 - W_{11}\Delta_2)}{2\{\tilde{\in}_1^2 - \tilde{\in}_2^2 + (W_{11}\Delta_1 + W_{12}\Delta_2)^2 - (W_{12}\Delta_1 + W_{11}\Delta_2)^2\}}$$

$$\left[\frac{1}{\sqrt{\tilde{\in}_1^2 + (W_{11}\Delta_1 + W_{12}\Delta_2)^2 + W_{12}^2\gamma^2}}\tanh\frac{1}{2k_BT}\sqrt{\tilde{\in}_1^2 + (W_{11}\Delta_1 + W_{12}\Delta_2)^2 + W_{12}^2\gamma^2}\right.$$

$$\left. - \frac{1}{\sqrt{\tilde{\in}_2^2 + (W_{12}\Delta_1 + W_{11}\Delta_2)^2 + W_{12}^2\gamma^2}}\tanh\frac{1}{2k_BT}\sqrt{\tilde{\in}_2^2 + (W_{12}\Delta_1 + W_{11}\Delta_2)^2 + W_{12}^2\gamma^2}\right]$$

(23)

$$< a_{2-k\downarrow} a_{2k\uparrow} >$$

$$= \frac{(W_{12}\Delta_1 + W_{11}\Delta_2)}{2\sqrt{\tilde{\in}_2^2 + (W_{12}\Delta_1 + W_{11}\Delta_2)^2 + W_{12}^2\gamma^2}} \tanh \frac{1}{2k_B T}\sqrt{\tilde{\in}_2^2 + (W_{12}\Delta_1 + W_{11}\Delta_2)^2 + W_{12}^2\gamma^2}$$

$$+ \frac{W_{12}^2\gamma^2 (W_{11}\Delta_1 + W_{12}\Delta_2 - W_{12}\Delta_1 - W_{11}\Delta_2)}{2\left\{\tilde{\in}_1^2 - \tilde{\in}_2^2 + (W_{11}\Delta_1 + W_{12}\Delta_2)^2 - (W_{12}\Delta_1 + W_{11}\Delta_2)^2\right\}}$$

$$\left[\frac{1}{\sqrt{\tilde{\in}_2^2 + (W_{12}\Delta_1 + W_{11}\Delta_2)^2 + W_{12}^2\gamma^2}} \tanh \frac{1}{2k_B T}\sqrt{\tilde{\in}_2^2 + (W_{12}\Delta_1 + W_{11}\Delta_2)^2 + W_{12}^2\gamma^2}\right.$$

$$\left. - \frac{1}{\sqrt{\tilde{\in}_1^2 + (W_{11}\Delta_1 + W_{12}\Delta_2)^2 + W_{12}^2\gamma^2}} \tanh \frac{1}{2k_B T}\sqrt{\tilde{\in}_1^2 + (W_{11}\Delta_1 + W_{12}\Delta_2)^2 + W_{12}^2\gamma^2}\right] \quad (24)$$

$$< a_{1k\uparrow} a_{1k\uparrow}^{+} > = -\frac{1}{2} + \frac{1}{2(\alpha_1^2 - \alpha_2^2)}\left\{\frac{W_{12}^2\gamma^2(\tilde{\in}_1 + \tilde{\in}_2)}{\alpha_2}\tanh\frac{\beta\alpha_2}{2}\right.$$

$$\left. - \frac{(\alpha_1^2 - \alpha_2^2)\tilde{\in}_1 + W_{12}^2\gamma^2(\tilde{\in}_1 + \tilde{\in}_2)}{\alpha_1}\tanh\frac{\beta\alpha_1}{2}\right\} \quad (25)$$

$$< a_{2k\uparrow} a_{2k\uparrow}^{+} > = -\frac{1}{2} + \frac{1}{2(\alpha_1^2 - \alpha_2^2)}\left\{\frac{\tilde{\in}_2(\alpha_2^2 - \alpha_1^2) + W_{12}^2\gamma^2(\tilde{\in}_1 + \tilde{\in}_2)}{\alpha_2}\tanh\frac{\beta\alpha_2}{2}\right.$$

$$\left. - \frac{W_{12}^2\gamma^2(\tilde{\in}_1 + \tilde{\in}_2)}{\alpha_1}\tanh\frac{\beta\alpha_1}{2}\right\} \quad (26)$$

3. Physical Properties

3.1 Superconducting Order Parameter:

The order parameters for superconducting state are given by [5, 24]

$$\Delta_a = W_{11}\Delta_1 = W_{11}\sum_k < a_{1-k\downarrow} a_{1k\uparrow} > \quad (27)$$

& $$\Delta_b = W_{11}\Delta_2 = W_{11}\sum_k < a_{2-k\downarrow} a_{2k\uparrow} > \quad (28)$$

Now for Δ_a, we use correlation function given by equation (23) & the summation over 'k' can be converted into integration using the relation.

$$\sum_k \rightarrow N(0) \int_{-\hbar\omega_D}^{+\hbar\omega_D} d\in_1$$

or $$\sum_k \rightarrow 2N(0) \int_0^{\hbar\omega_D} d\in_1 \tag{29}$$

Using $\Delta_b = 0$, $\in_2 = 0$, & neglecting W_{12}^2 in comparison to W_{11}^2, finally we get

$$\Delta_a = N(0)\int_0^{\hbar\omega_D} d\in_1 \left[\frac{\Delta_a \tanh \frac{1}{2k_\beta T}\sqrt{\tilde{\in}_1^2 + \Delta_a^2 + W_{12}^2\gamma^2}}{\sqrt{\tilde{\in}_1^2 + \Delta_a^2 + W_{12}^2\gamma^2}} + \frac{W_{12}^2\gamma^2\Delta_a\left(1-\frac{W_{12}}{W_{11}}\right)}{\tilde{\in}_1^2 - \frac{W_{11}^2}{4} + W_{11}^2\Delta_1^2} \right.$$

$$\left. \left\{ \frac{\tanh \frac{1}{2k_\beta T}\sqrt{\tilde{\in}_1^2 + \Delta_a^2 + W_{12}^2\gamma^2}}{\sqrt{\tilde{\in}_1^2 + \Delta_a^2 + W_{12}^2\gamma^2}} - \frac{\tanh \frac{1}{2k_\beta T}\sqrt{\frac{W_{11}^2}{4} + \left(\frac{W_{12}^2}{W_{11}^2}\right)\Delta_a^2 + W_{12}^2\gamma^2}}{\sqrt{\frac{W_{11}^2}{4} + \left(\frac{W_{12}^2}{W_{11}^2}\right)\Delta_a^2 + W_{12}^2\gamma^2}} \right\} \right] \tag{30}$$

Thus, we obtain self-consistent equation for superconducting order parameter Δ_a as

$$\frac{1}{N(0)} = \int_0^{\hbar\omega_D} \frac{\tanh \frac{1}{2k_\beta T}\sqrt{\left(\in_1 - \frac{W_{11}}{2}\right)^2 + \Delta_a^2 + W_{12}^2\gamma^2}}{\sqrt{\left(\in_1 - \frac{W_{11}}{2}\right)^2 + \Delta_a^2 + W_{12}^2\gamma^2}} d\in_1$$

$$+ W_{12}^2\gamma^2\left(1-\frac{W_{12}}{W_{11}}\right)\int_0^{\hbar\omega_D} \frac{1}{\left\{\left(\in_1 - \frac{W_{11}}{2}\right)^2 + \Delta_a^2 - \frac{W_{11}^2}{4}\right\}} \frac{\tanh \frac{1}{2k_\beta T}\sqrt{\left(\in_1 - \frac{W_{11}}{2}\right)^2 + \Delta_a^2 + W_{12}^2\gamma^2}}{\sqrt{\left(\in_1 - \frac{W_{11}}{2}\right)^2 + \Delta_a^2 + W_{12}^2\gamma^2}} d\in_1$$

$$- \frac{W_{12}^2\gamma^2\left(1-\frac{W_{12}}{W_{11}}\right)\tanh \frac{1}{2k_\beta T}\sqrt{\frac{W_{11}^2}{4} + \frac{W_{12}^2}{W_{11}^2}\Delta_a^2 + W_{12}^2\gamma^2}}{\sqrt{\frac{W_{11}^2}{4} + \frac{W_{12}^2}{W_{11}^2}\Delta_a^2 + W_{12}^2\gamma^2}} \times \int_0^{\hbar\omega_D} \frac{d\in_1}{\left(\in_1 - \frac{W_{11}}{2}\right)^2 - \frac{W_{11}^2}{4} + \Delta_a^2}$$

(31)

To derive an expression for Δ_b we use correlation function (Eq. 24). Following the same procedure, we obtain self-consistent equation for order parameter Δ_b as

$$\frac{1}{N(0)} = \int_0^{\hbar\omega_D} \frac{\tanh \frac{1}{2k_\beta T}\sqrt{\left(\epsilon_2 - \frac{W_{11}}{2}\right)^2 + \Delta_b^2 + W_{12}^2\gamma^2}}{\sqrt{\left(\epsilon_2 - \frac{W_{11}}{2}\right)^2 + \Delta_b^2 + W_{12}^2\gamma^2}} d\epsilon_2$$

$$+W_{12}^2\gamma^2\left(1-\frac{W_{12}}{W_{11}}\right)\int_0^{\hbar\omega_D} \frac{d\epsilon_2}{\left\{\left(\epsilon_2 - \frac{W_{11}}{2}\right)^2 + \Delta_b^2 - \frac{W_{11}^2}{4}\right\}} \frac{\tanh \frac{1}{2k_B T}\sqrt{\left(\epsilon_2 - \frac{W_{11}}{2}\right)^2 + \Delta_b^2 + W_{12}^2\gamma^2}}{\sqrt{\left(\epsilon_2 - \frac{W_{11}}{2}\right)^2 + \Delta_b^2 + W_{12}^2\gamma^2}}$$

$$-W_{12}^2\gamma^2\left(1-\frac{W_{12}}{W_{11}}\right) \frac{\tanh \frac{1}{2k_\beta T}\sqrt{\frac{W_{11}^2}{4} + \frac{W_{12}^2}{W_{11}^2}\Delta_b^2 + W_{12}^2\gamma^2}}{\sqrt{\frac{W_{11}^2}{4} + \frac{W_{12}^2}{W_{11}^2}\Delta_b^2 + W_{12}^2\gamma^2}} \int_0^{\hbar\omega_D} \frac{d\epsilon_2}{\left(\epsilon_2 - \frac{W_{11}}{2}\right)^2 + \Delta_b^2 - \frac{W_{11}^2}{4}}$$

(32)

With the help of self-consistent equations (31) and (32), we can study the temperature dependence of superconducting order parameter.

3.2 Electronic Specific Heat (C_{es}):

The electronic specific heat per atom of a superconductor is determined from the following relation [16,21-24]

$$C_{es} = \frac{\partial}{\partial T}\left[\frac{1}{N}\sum_k 2\epsilon_k < a_{k\uparrow} a_{k\uparrow}^{+} >\right] \quad (33)$$

Here $< a_{k\uparrow} a_{k\uparrow}^{+} >$ is the correlation function.

The expression for electronic specific heat "$C_{es}^{(1)}$" -

$$C_{es}^{(1)} = \frac{1}{N}\frac{\partial}{\partial T}\left[\sum_k 2\epsilon_1 < a_{1k\uparrow} a_{1k\uparrow}^{+} >\right] \quad (34)$$

Changing summation over k into integration by using the relation (29) and using the correlation function equation (25) and writing $\Delta_b = 0$ and $\epsilon_2 = 0$ and solving, we get

$$C_{es}^{(1)} = \frac{N(0)}{N}\frac{1}{2k_B T^2}\left[\int \epsilon_1\left(\left(\epsilon_1 - \frac{W_{11}}{2}\right)\sec h^2 \frac{1}{2k_B T}\sqrt{\left(\epsilon_1 - \frac{W_{11}}{2}\right)^2 + \Delta_a^2 + W_{12}^2\gamma^2}\cdot d\epsilon_1\right)\right.$$

$$+W_{12}^2\gamma^2 \int \epsilon_1 \left(\frac{(\epsilon_1 - W_{11})\cdot \sec h^2 \frac{1}{2k_B T}\sqrt{\left(\epsilon_1 - \frac{W_{11}}{2}\right)^2 + \Delta_a^2 + W_{12}^2\gamma^2}}{\epsilon_1^2 - \epsilon_1 W_{11} + \Delta_a^2} d\epsilon_1\right)$$

$$\left. -W_{12}^2\gamma^2 \sec h^2 \frac{1}{2k_B T}\sqrt{\frac{W_{11}^2}{4} + \frac{W_{12}^2}{W_{11}^2}\Delta_a^2 + W_{12}^2\gamma^2}\left(\int \frac{\epsilon_1(\epsilon_1 - W_{11})}{\epsilon_1^2 - \epsilon_1 W_{11} + \Delta_a^2} d\epsilon_1\right)\right] \tag{35}$$

Here $\beta = \frac{1}{k_B T}$

Similarly the expression for electronic specific heat "$C_{es}^{(2)}$" -

$$C_{es}^{(2)} = \frac{N(0)}{N}\cdot\frac{1}{2k_B T^2}\left[\int \epsilon_2\left(\epsilon_2 - \frac{W_{11}}{2}\right)\sec h^2 \frac{1}{2k_B T}\sqrt{\left(\epsilon_2 - \frac{W_{11}}{2}\right)^2 + \Delta_b^2 + W_{12}^2\gamma^2}\cdot d\epsilon_2\right.$$

$$+W_{12}^2\gamma^2 \int \epsilon_2 \frac{(\epsilon_2 - W_{11})\cdot \sec h^2 \frac{1}{2k_B T}\sqrt{\left(\epsilon_2 - \frac{W_{11}}{2}\right)^2 + \Delta_b^2 + W_{12}^2\gamma^2}}{\epsilon_2^2 - \epsilon_2 W_{11} + \Delta_b^2} d\epsilon_2$$

$$\left. -W_{12}^2\gamma^2 \sec h^2 \frac{1}{2k_B T}\sqrt{\frac{W_{11}^2}{4} + \frac{W_{12}^2}{W_{11}^2}\Delta_b^2 + W_{12}^2\gamma^2}\int \frac{\epsilon_2(\epsilon_2 - W_{11})}{\epsilon_2^2 - \epsilon_2 W_{11} + \Delta_b^2} d\epsilon_2\right] \tag{36}$$

4. Results:

Values of various parameters appearing in equations obtained in section 3 are given in Table 1.Using these values we have made study of various properties for MgB_2.

(i) Superconducting Order Parameter $(\Delta = \Delta_a + \Delta_b)$

Our model exhibit two superconducting gaps, Δ_a and Δ_b $(\Delta = \Delta_a + \Delta_b)$. Using the values of various parameters given in Table 1 in equation (31), we obtain the temperature dependence of gap parameter, Δ for different values of matrix element of interband interaction W_{12} as shown in Figs. 1 and 2. Our results agree well with experimental data [17, 18].

(ii) Electronic Specific Heat: $(C_{es} = C_{es}^{(1)} + C_{es}^{(2)})$

Temperature dependence of electronic specific heat $(C_{es} = C_{es}^{(1)} + C_{es}^{(2)}$, where $C_{es}^{(1)}$ and $C_{es}^{(2)}$ are specific heats corresponding to gap parameters Δ_a and Δ_b respectively $)$ obtained from equations (36) and (37) for different values of matrix element W_{12} are shown in Figs. 3 and 4. For comparison, experimental curve is also shown [29]. The agreement between theory and experimental results is quite encouraging.

5. Conclusions:

From the above results we draw following inferences:

(1) The superconducting order parameter Δ decreases slightly with the increase in the value of matrix element of interband interaction W_{12}. The general behaviour of Δ as a function of temperature is slightly different from the behaviour of BCS predictions. This is expected due to highly anisotropic nature of MgB_2.The presence of the two gap structure observed experimentally is in good agreement with our model.

(2) The electronic specific heat C_{es} slightly increases with the increase in the value of matrix element of interband interaction (W_{12}). This is also due to anisotropic nature

In summary, we studied the superconducting order parameter and, electronic specific heat of superconductor MgB_2 based on the two – band model with intra- and interband interactions. We have derived the temperature dependences of two superconducting gaps. Our results agree well with the experimental data for superconducting order parameter and electronic specific heat. The study strongly supports the existence of two band superconductivity with intra- and interband interactions in MgB_2.

6. References:

1. J. Nagamatsu, N. Nakagawa, T. Muranaka, Y. Zenitani, J. Akimitsu, Nature 410, 63 (2001) .
2. P. Grant, Nature 411,532 (2001) .
3. A. M. Campbell, Science 292, 65 (2001).
4. S. L. Kakani, S. Kakani, Superconductivity, (New Age International Publishers, New Delhi-2, 2017), pp 459-545.
5. Sergey. L. Bud'ko, Paul C. Canfield, Physica C 514 , 142 (2015) .
6. J. M. An, W. E. Pickett, Phys. Rev. Lett. , 86, 4366 (2001).
7. J. Kortus, I. I. Mazin, K. D. Belaschenko, V. P. Antropov, L. L. Boyer, Phys. Rev. Lett. 86, 4656 (2001).
8. Morton E. Jones, Richard E. Marsh, J. Am. Chem. Soc. 76, 1434 (1954).
9. A. Y. Liu, Y. Y. Mazin, Y. Kortus, Phys. Rev. Lett., 87, 087005 (2001).
10. A. Kristoffel, T. Ord, K. Rago, Europhys. Lett., 61 ,109 (2003).
11. A. Bussmann-Holder, A. Bianconi, Phys. Rev. B 67, 132509 (2003).
12. R. Klenier, W. Buckel, Superconductivity: An Introduction,3rd edn.,(Wiley-VCH Verlag GmbH and Co. KGaA - Germany, 2016), pp 283-295.
13. M. Iavarone, G. Karapetrov, A.E. Koshelev, W.K. Kwok, G.W. Crabtree, D.G. Hinks, W.N. Kang, E.M. Choi, H.J. Kim, S.I. Lee, Phys. Rev. Lett.89, 187002 (2002).
14. F.Giubileo, D. Roditchev, W. Sacks, R. Lamy, D. X. Thanh, J. Klein, S. Miraglia, D. Fruchart, J. Marcus, Ph. Monod, Phys. Rev. Lett. 87, 177008 (2001) .
15. P. Szabó, P. Samuely, J. Kačmarčík, T. Klein, J. Marcus, D. Fruchart, S. Miraglia, C. Marcenat, A. G. M. Jansen: Phys. Rev. Lett. 87, 137005 (2001).
16. H. J. Choi, D. Roundy, H. Sun, M. L. Cohen, S. G. Louie, Nature, 418,758 (2002).
17. K. H. Bennemann, J. B. Ketterson, Superconductivity Vol. 1, (Springer-Verlag, Berlin Heidelberg, 2008), pp 3-153.
18. X. X. Xi, Rep. Prog. Phys., 71, 116501 (2008).
19. K. P. Bohnen, R. Heid, B. Renker, Phys. Rev. Lett., 86 , 5771 (2001).

20. A. Vargunin, T. Ord , K. Rago , J. Supercond. Nov. Magn. 24, 1127 (2011).
21. S. L. Kakani, U. N. Upadhyaya, J. Low Temp. Phys, 53, 221 (1983).
22. S. L. Kakani , U. N. Upadhyaya, Phys. Stat. Sol. (b), 125, 861 (1984).
23. S. L. Kakani, U. N. Upadhyaya, Phys. Stat. Sol. (a), 99,15 (1987).
24. S. L. Kakani, U. N. Upadhyaya, J. Low Temp. Phys, 70, 5 (1988).
25. D. N. Zubarev, Usp. Fiz. Nauk. SSSR, 71, 71 (1960 a) .
26. D. N. Zubarev, Sov. Phys. Usp., 3, 320 (1960 b).
27. Y. Takada, Phys. Rev. B, 43, 6124 (1991).
28. Y. Takada, Y. Kohmoto, Phys. Rev. B, 41, 8872 (1990).
29. C. H. Walti, E. Felder,C. Degen , G. Wigger , R. Monnier , B. Delley and H. R. Ott, Phys. Rev. B 64 , 172515 (2001).
30. G. Alecu, Romanian Reports in Physics, Vol. 56, No. 3,404 (2004).
31. A. Kashyap , S.C. Tiwari , A. Surana , R. K. Paliwal , S. L. Kakani, Journal of Superconductivity and Novel Magnetism, 21, 129 (2004).

Table 1

No.	Parameter	Value	References
.	nducting transition temperature T_c	39 K	1,2
.	energy ε_1	0.06 eV	5,17
.	energy ε_2	0.05 eV	5,17
.	states at the Fermi surface N(0)	)93/ eV. atom	1,2
.	nteraction $W_{11} = W_{22}$ intra-band	0.3 eV. cell	20
.	nteraction $W_{12} = W_{21}$ inter-band	).01eV. cell 0.1 eV. cell	20
.	toms per unit volume N	$5\times10^{28}/m^3$	31
.	ameters for MgB_2	$a = 3.086\ A^0$ $b = 3.524\ A^0$	30
.	nn's constant (k_B)	$1.38\times10^{-23}\ J/K$	-
).	electron m_e	$9.1\times10^{-31}\ kg.$	-

Values of Various Parameters for MgB_2

Table 2

Superconducting Order Parameter Δ for MgB_2 system

No.	mperature (K)	Δ Theoretical (in meV)		Δ imental (in meV)
		= 0.01 eV.cell	= 0.1 eV.cell	
1	0	11.4147	11.4135	10.10
2	5	11.4147	11.4135	10.10
3	10	11.3974	11.3962	10.02
4	15	11.2301	11.2290	9.75
5	20	10.7274	10.7266	9.10
6	25	9.7242	9.7190	7.90
7	30	7.9289	7.9286	5.85
8	35	3.9766	4.0062	3.18
9	39	0.0120	0.1200	0.00

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Table 3

Electronic Specific Heat C_{es} for MgB_2 system

o.	mperature (K)	nic Specific heat Theoretical (in 10^{-49} J)		tronic Specific heat mental (in 10^{-49} J)
		= 0.01 eV.cell	= 0.1 eV.cell	
	5	0.00027	0.00028	1.90
	10	0.46861	0.47076	10.10
	15	4.90098	4.91015	29.10
	20	15.94030	15.95743	45.30
	25	33.43365	33.47148	64.00
	30	56.55598	56.52985	91.80
	35	84.26450	84.21433	113.90
	39	101.19994	103.14835	101.20

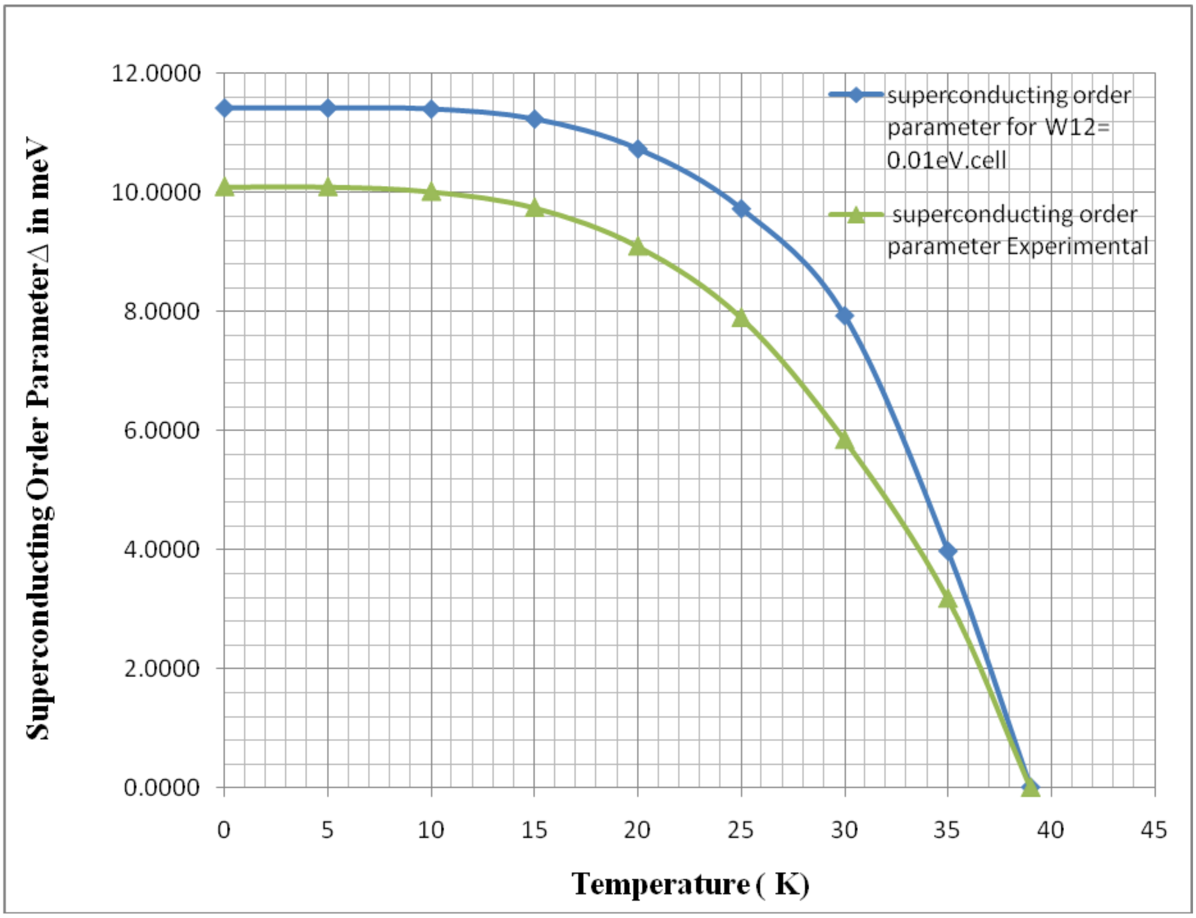

Fig. 1 Temperature dependence of superconducting order parameter Δ for W_{12} =0.01 eV.cell

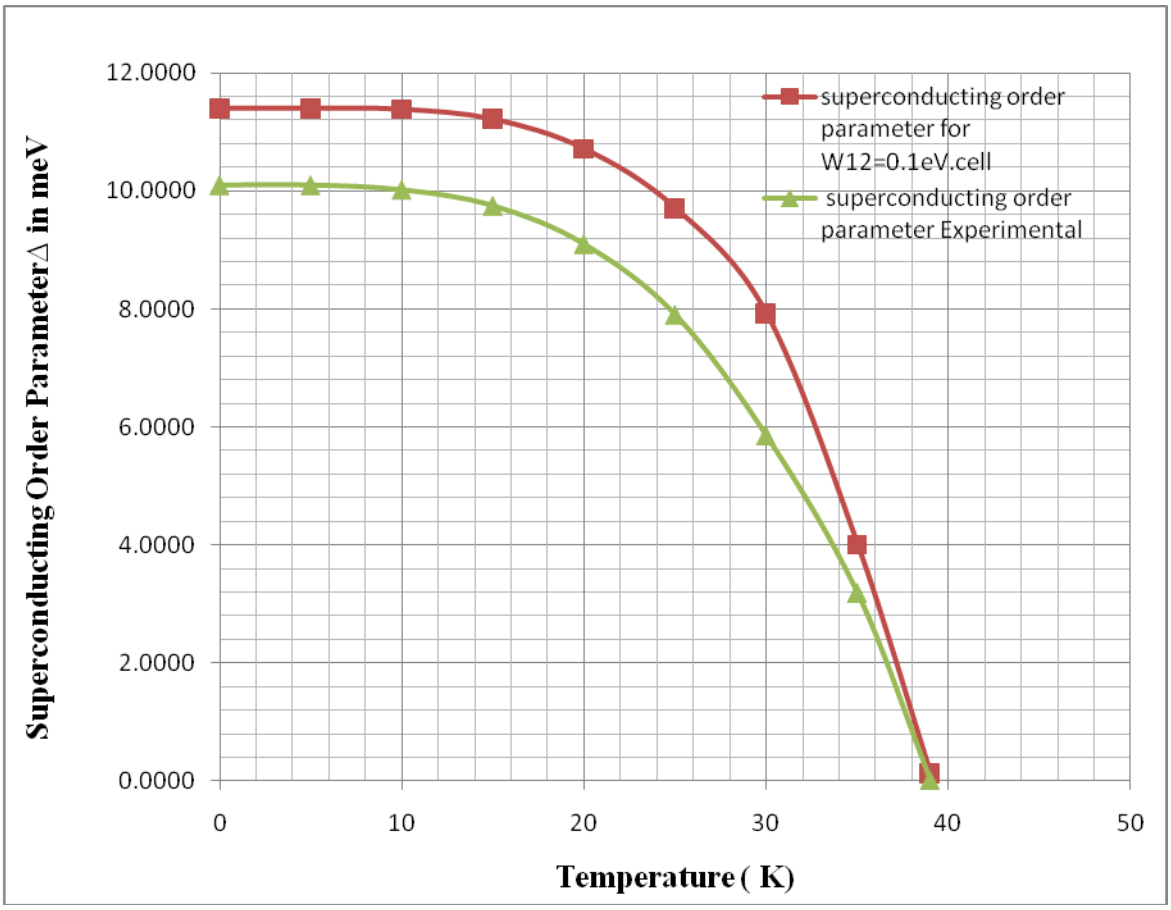

Fig. 2 Temperature dependence of superconducting order parameter Δ for W_{12} =0.1 eV.cell

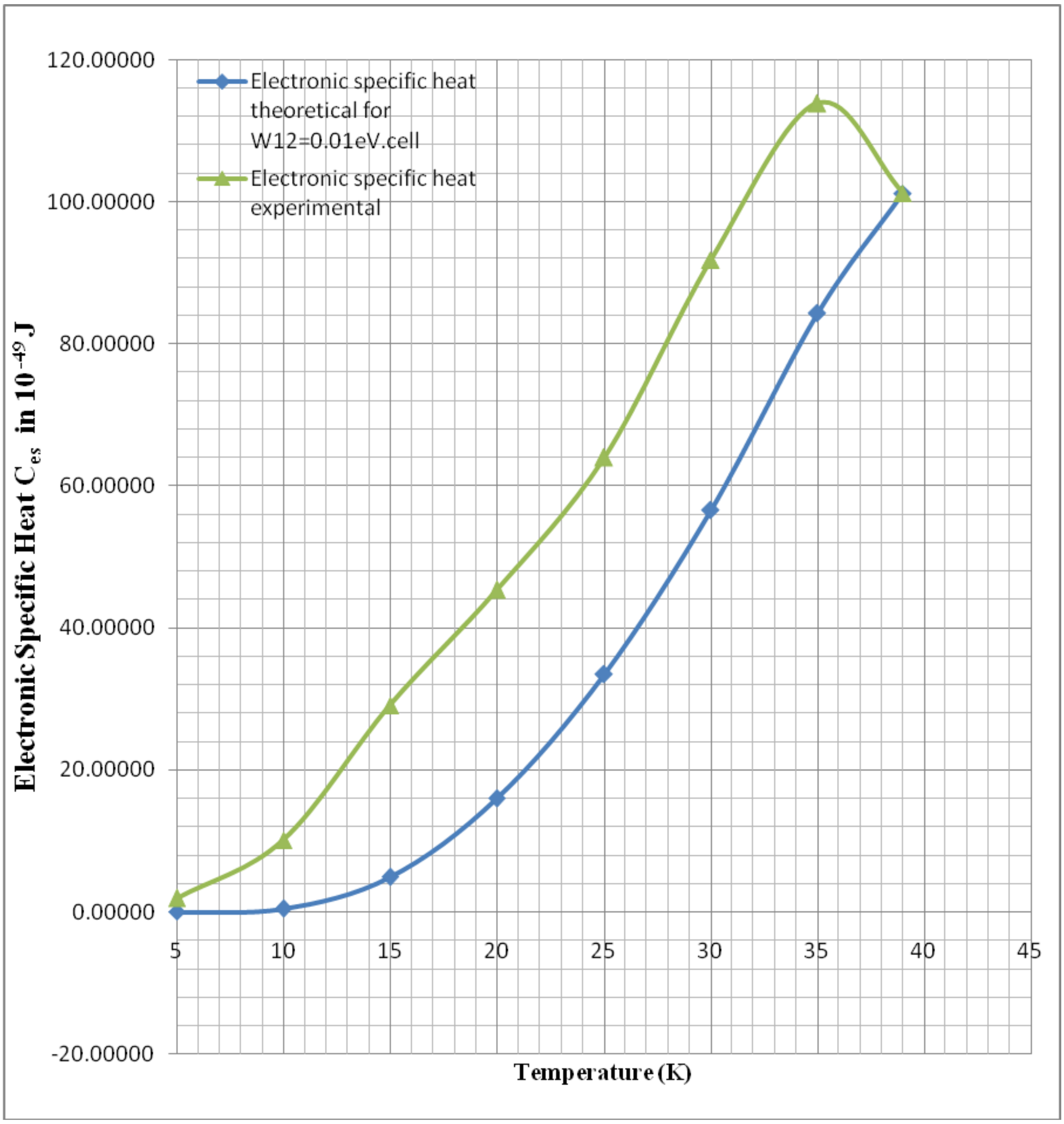

Fig. 3 Temperature dependence of Electronic specific heat for W12 =0.01 eV.cell

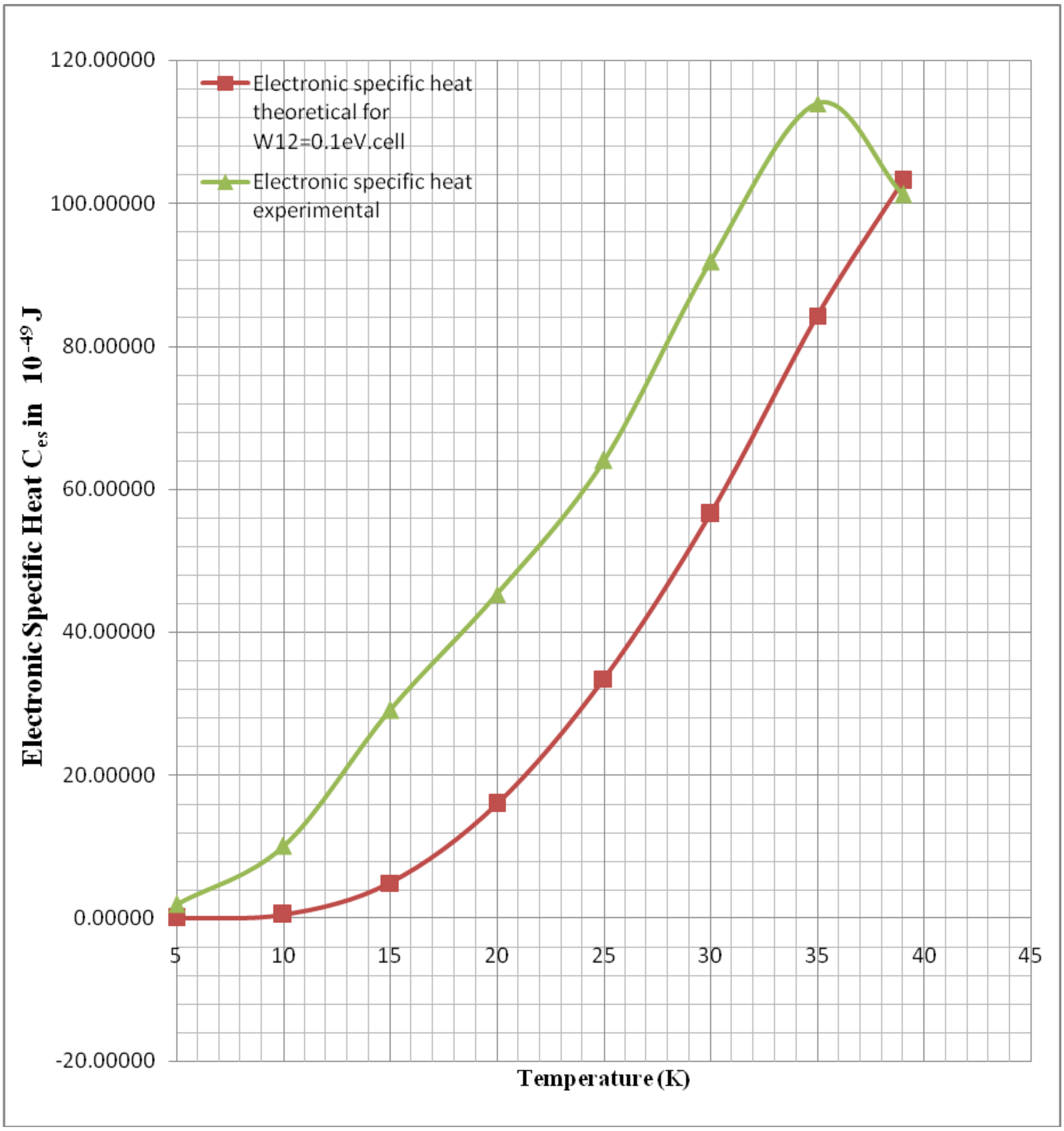

Fig. 4 Temperature dependence of Electronic specific heat for W_{12} =0.1 eV.cell