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THEORETICAL STUDY OF SPECIFIC HEAT OF MAGNESIUM DIBORIDE SUPERCONDUCTOR BASED ON MULTIBAND MODEL

PRADEEP CHAUDHARY*, R. K. PALIWAL and S. C. TIWARI[a]

Department of Physics, Mewar University, Gangrar, CHITTORGARH (Raj.) INDIA
[a]Department of Physics, M. L. V. Govt. College, BHILWARA (Raj.) INDIA

ABSTRACT

Magnesium diboride with T_c = 39 K is a record breaking compound among s-p metals and alloys. Many experiments performed on magnesium diboride suggest that there are two superconducting gaps. Considering a multiband model Hamiltonian with intra- and inter band pair transfer interactions, we have derived the normal and anomalous one-particle green's function and self consistent equations for superconducting order parameter (Δ) using green's function technique and equation of motion method. The study of electronic specific heat is also presented. The agreement between theoretical and experimental results for electronic specific heat is quite satisfactory.

Key words: Two band superconductivity, Hamiltonian, Green's functions, Superconducting order parameter, Electronic specific heat.

INTRODUCTION

Magneisum diboride is an old material, known since early 1950's but it was discovered to be a superconductor by Nagamatsu et al.[1] at a remarkably high temperature about 39 K. This discovery certainly received the attention of many researchers in the field of superconductivity especially in non oxides and initiated a search for superconductivity in related boron compounds[2].

Magnesium diboride is receiving attention due to exceptionally high values of critical temperature and critical field. This material may be suitable contender to replace Nb_3Sn or NbTi as the choice for practical large scale application in the range of 20-30 K operating with cryogenic refrigerators.

*Author for correspondence; E-mail: pchaudhary45@gmail.com, sct_123@rediff.com

MgB_2 possesses the simple hexagonal AlB_2 type structure. It contains graphite type boron layers, which are separated by closed packed layers of magnesium. Magnesium atoms are located at the centre of hexagons formed by borons. Band structure calculation of MgB_2 reveals that there are two types of bands with two superconducting gaps in the excitation spectrum at the Fermi surface. The first one is a heavy hole band built up of σ band orbital and the second one is the broader band built up mainly of π band orbital[3-7].

It is an established fact that MgB_2 is an anisotropic two gap superconductor[4]. Both the energy gaps have s-wave symmetries; the larger gap is highly anisotropic while the smaller one is slightly anisotropic. It is natural to describe a two gap superconductor by means of a two band model with inter band coupling[8,9]. Malik and Malik[10] have presented a detailed study of the thermal conductivity of MgB_2 in the superconducting state. Nik-Jaafar et al.[11] calculated the electron-phonon coupling constant within the BCS framework and the two dimensional van Hove scenario. They concluded that MgB_2 is a moderately-strong coupled superconductor.

For MgB_2, an approach of such kind is also directly proposed by the nature of electron spectrum mentioned. There is a number of two band type approaches for superconductivity in magnesium diboride[12]. Two band models have been exploited in various realisations for cuprate superconductivity. Liu et al.[4] pointed out the role of electron-phonon interaction between σ and π bands in magnesium diboride.

Using two band model, we have studied the superconducting order parameter and electronic specific heat of magnesium diboride and compared the theoretical results with available experimental data.

Model Hamiltonian

We start with two band Hamiltonian with intra- and inter-band pair transfer interactions[13].

$$H = \sum_{\alpha ls} \bar{\epsilon}_\alpha(l) a^+_{\alpha ls} a_{\alpha ls} - \frac{1}{V}\sum_{\alpha\alpha'}\sum_{lm} W_{\alpha\alpha'}(l,m) a^+_{\alpha l\uparrow} a^+_{\alpha -l\downarrow} a_{\alpha' -m\downarrow} a_{\alpha' m\uparrow} \qquad \ldots(1)$$

Where $\bar{\epsilon}_\alpha = \epsilon_\alpha - \mu$ is the electron energy in the bands $\alpha = 1,2$; μ is the chemical potential; V is the volume of the superconductor and $w_{\alpha\alpha'}(l, m)$ are the matrix elements of intra-band or inter-band interactions, if $\alpha = \alpha'$ or $\alpha \neq \alpha'$, respectively.

Final Hamiltonian can be written as –

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

where

$$H_{11} = \sum_{ls} \in_1 (l) a^{+}_{1ls} a_{1ls} - \frac{1}{V} \sum_{lm} W_{11}(lm) a^{+}_{1l\uparrow} a^{+}_{1-l\downarrow} a_{1-m\downarrow} a_{1m\uparrow}$$

$$H_{22} = \sum_{ls} \in_2 (l) a^{+}_{2ls} a_{2ls} - \frac{1}{V} \sum_{lm} W_{22}(lm) a^{+}_{2l\uparrow} a^{+}_{2-l\downarrow} a_{2-m\downarrow} a_{2m\uparrow}$$

$$H_{12} = \sum_{ls} \in_1 (l) a^{+}_{1ls} a_{1ls} - \frac{1}{V} \sum_{lm} W_{12}(lm) a^{+}_{1l\uparrow} a^{+}_{1-l\downarrow} a_{2-m\downarrow} a_{2m\uparrow}$$

$$H_{21} = \sum_{ls} \in_2 (l) a^{+}_{2ls} a_{2ls} - \frac{1}{V} \sum_{lm} W_{21}(lm) a^{+}_{2l\uparrow} a^{+}_{2-l\downarrow} a_{1-m\downarrow} a_{1m\uparrow} \quad \ldots(3)$$

On solving, one obtain

$$[a_{1k\uparrow}, H] = \in_1 (k) a_{1k\uparrow} - \frac{1}{V} \sum_m W_{11}(k,m) a^{+}_{1-k\downarrow} a_{1-m\downarrow} a_{1m\uparrow} - \frac{1}{V} \sum_m W_{12}(k,m) a^{+}_{1-k\downarrow} a_{2-m\downarrow} a_{2m\uparrow} \quad \ldots(4)$$

$$[a_{2k\uparrow}, H] = \in_2 (k) a_{2k\uparrow} - \frac{1}{V} \sum_m W_{22}(k,m) a^{+}_{2-k\downarrow} a_{2-m\downarrow} a_{2m\uparrow} - \frac{1}{V} \sum_m W_{21}(k,m) a^{+}_{2-k\downarrow} a_{1-m\downarrow} a_{1m\uparrow} \quad \ldots(5)$$

$$[a^{+}_{1-k\downarrow}, H] = - \in_1 (-k) a^{+}_{1-k\downarrow} - \frac{1}{V} \sum_l W_{11}(l,k) a^{+}_{1l\uparrow} a^{+}_{1-l\downarrow} a_{1k\uparrow} - \frac{1}{V} \sum_l W_{21}(l,k) a^{+}_{2l\uparrow} a^{+}_{2-l\downarrow} a_{1k\uparrow} \quad \ldots(6)$$

$$[a^{+}_{2-k\downarrow}, H] = - \in_2 (-k) a^{+}_{2-k\downarrow} - \frac{1}{V} \sum_l W_{22}(l,k) a^{+}_{2l\uparrow} a^{+}_{2-l\downarrow} a_{2k\uparrow} - \frac{1}{V} \sum_m W_{12}(l,k) a^{+}_{1l\uparrow} a^{+}_{1-l\downarrow} a_{2k\uparrow} \quad \ldots(7)$$

Green's functions

In order to study the physical properties, we define following normal & anomalous Green's functions as follows[14-24]:

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

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

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

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

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

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

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

$$F_{22}(2,k,\uparrow)=\left\langle\left\langle a^{+}_{2-k\downarrow} \mid a^{+}_{2k\uparrow}\right\rangle\right\rangle \qquad \ldots(8)$$

On solving, one get

$$\left[\omega-\tilde{\in}_1(k)\right]G_{11}=1-W_{12}\gamma_{12}G_{21}-\left[W_{11}\Delta_{11}+W_{12}\Delta_{22}\right]F_{11}$$

$$\left[\omega-\tilde{\in}_2(k)\right]G_{22}=1-W_{12}\gamma_{21}G_{12}-\left[W_{12}\Delta_{11}+W_{22}\Delta_{22}\right]F_{22}$$

$$\left[\omega-\tilde{\in}_2(k)\right]G_{21}=1-W_{12}\gamma_{21}G_{11}-\left[W_{12}\Delta_{11}+W_{22}\Delta_{22}\right]F_{21}$$

$$\left[\omega-\tilde{\in}_1(k)\right]G_{12}=1-W_{12}\gamma_{12}G_{22}-\left[W_{11}\Delta_{11}+W_{12}\Delta_{22}\right]F_{12}$$

$$\left[\omega+\tilde{\in}_1(-k)\right]F_{11}=W_{21}\gamma_{21}F_{21}-\left[W_{11}\Delta^{+}_{11}+W_{21}\Delta^{+}_{22}\right]G_{11}$$

$$\left[\omega+\tilde{\in}_2(-k)\right]F_{22}=W_{12}\gamma_{12}F_{12}-\left[W_{12}\Delta^{+}_{11}+W_{22}\Delta^{+}_{22}\right]G_{22}$$

$$\left[\omega+\tilde{\in}_2(-k)\right]F_{21}=W_{12}\gamma_{12}F_{11}-\left[W_{12}\Delta^{+}_{11}+W_{22}\Delta^{+}_{22}\right]G_{21}$$

$$\left[\omega+\tilde{\in}_1(-k)\right]F_{12}=W_{21}\gamma_{21}F_{22}-\left[W_{11}\Delta^{+}_{11}+W_{21}\Delta^{+}_{22}\right]G_{12} \qquad \ldots(9)$$

Where

$$\tilde{\in}_1(k)=\overline{\in}_1(k)-W_{11}n_{1-k\downarrow} \qquad n_{1-k\downarrow}=\frac{1}{V}\left\langle a^{+}_{1-k\downarrow}a_{1-k\downarrow}\right\rangle$$

$$\tilde{\in}_2(k)=\overline{\in}_2(k)-W_{22}n_{2-k\downarrow} \qquad n_{2-k\downarrow}=\frac{1}{V}\left\langle a^{+}_{2-k\downarrow}a_{2-k\downarrow}\right\rangle$$

$$\tilde{\epsilon}_1(-k) = \bar{\epsilon}_1(-k) - W_{11} n_{1k\uparrow} \qquad n_{1k\uparrow} = \frac{1}{V}\left\langle a^{+}_{1k\uparrow} a_{1k\uparrow} \right\rangle$$

$$\tilde{\epsilon}_2(-k) = \bar{\epsilon}_2(-k) - W_{22} n_{2k\uparrow} \qquad n_{2k\uparrow} = \frac{1}{V}\left\langle a^{+}_{2k\uparrow} a_{2k\uparrow} \right\rangle$$

$$\gamma_{12} = \frac{1}{V}\left\langle a^{+}_{1-k\downarrow} a_{2-k\downarrow} \right\rangle \qquad \gamma_{21} = \frac{1}{V}\left\langle a^{+}_{2-k\downarrow} a_{1-k\downarrow} \right\rangle$$

$$\Delta_{11} = \frac{1}{V}\left\langle a_{1-k\downarrow} a_{1k\uparrow} \right\rangle \qquad \Delta^{+}_{11} = \frac{1}{V}\left\langle a^{+}_{1k\uparrow} a^{+}_{1-k\downarrow} \right\rangle$$

$$\Delta_{22} = \frac{1}{V}\left\langle a_{2-k\downarrow} a_{2k\uparrow} \right\rangle \qquad \Delta^{+}_{22} = \frac{1}{V}\left\langle a^{+}_{2k\uparrow} a^{+}_{2-k\downarrow} \right\rangle$$

Solving G_{11} and F_{11} from Eq. (9) and using equation of motion method, we obtain Green's functions as follows. In obtaining Green's functions, we have assumed

$W_{12} = W_{21}$

$W_{11} = W_{22}$

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

$$\Delta_{11} = \Delta^{+}_{11} = \Delta_1 \;\&\; \Delta_{22} = \Delta^{+}_{22} = \Delta_2 \qquad \ldots(10)$$

$$G_{11} = \frac{\left[(\omega + \tilde{\epsilon}_1)\left\{(\omega^2 - \tilde{\epsilon}_2^2) - (W_{12}\Delta_1 + W_{11}\Delta_2)^2 - (\omega + \tilde{\epsilon}_2)W_{12}\gamma\right\} - (\omega - \tilde{\epsilon}_2)W_{12}^2\gamma^2\right]}{2\pi\left[(\omega^2 - \tilde{\epsilon}_1^2)(\omega^2 - \tilde{\epsilon}_2^2) - (\omega^2 - \tilde{\epsilon}_1^2)(W_{12}\Delta_1 + W_{11}\Delta_2)^2 - (\omega^2 - \tilde{\epsilon}_2^2)(W_{11}\Delta_1 + W_{12}\Delta_2)^2 - 2W_{12}^2\gamma^2(\omega^2 + \tilde{\epsilon}_1\tilde{\epsilon}_2)\right]} \qquad \ldots(11)$$

On further simplification, one obtain

$$G_{11} = \frac{1}{4\pi\alpha_1\alpha_2^2(\alpha_1^2 - \alpha_2^2)}\left[\frac{X + Y}{(\omega - \alpha_1)} + \frac{X - Y}{(\omega + \alpha_1)}\right] + \frac{W_{12}\gamma}{4\pi\alpha_2(\alpha_1^2 - \alpha_2^2)}\left[\frac{X_1 + Y_1}{(\omega - \alpha_2)} + \frac{X_1 - Y_1}{(\omega + \alpha_2)}\right] \qquad \ldots(12)$$

Where

$$X = \alpha_1^3\alpha_2^2 - \alpha_1\alpha_2^4 - \alpha_1\alpha_2^2 W_{12}\gamma\,\tilde{\epsilon}_1 - \alpha_1\alpha_2^2 W_{12}\gamma\,\tilde{\epsilon}_2 + \alpha_1\alpha_2^2 W_{12}^2\gamma^2$$

$$Y = (\alpha_1^2 - \alpha_2^2)\tilde{\epsilon}_1\left\{\tilde{\epsilon}_2^{\,2} + (W_{12}\Delta_1 + W_{11}\Delta_2)^2\right\} - \alpha_2^2\,\tilde{\epsilon}_1\tilde{\epsilon}_2\,W_{12}\gamma + \alpha_2^2\,\tilde{\epsilon}_2\,W_{12}^2\gamma^2 - 2\alpha_1^2 W_{12}^3\gamma^3$$
$$+ 2\alpha_1^2\,\tilde{\epsilon}_1\,W_{12}^2\gamma^2 - \alpha_1^2\,\tilde{\epsilon}_2^{\,2}\,W_{12}\gamma - \alpha_1^2 W_{12}\gamma(W_{12}\Delta_1 + W_{11}\Delta_2)^2$$

$$X_1 = \alpha_2(\tilde{\epsilon}_1 + \tilde{\epsilon}_2 - W_{12}\gamma)$$

$$Y_1 = \alpha_2^2 - W_{12}\gamma(\tilde{\epsilon}_2 + 2\,\tilde{\epsilon}_1) + \tilde{\epsilon}_1\tilde{\epsilon}_2$$

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

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

Similiarly

$$F_{11} = -\frac{\left[\begin{array}{l}(\omega + \tilde{\in}_2)(W_{11}\Delta_1 + W_{12}\Delta_2)(\omega - \tilde{\in}_2 - W_{12}\gamma) + (\omega - \tilde{\in}_1)W_{12}\gamma \\ (W_{12}\Delta_1 + W_{11}\Delta_2)\end{array}\right]}{2\pi\left[\begin{array}{l}(\omega^2 - \tilde{\in}_1^2)(\omega^2 - \tilde{\in}_2^2) - (\omega^2 - \tilde{\in}_1^2)(W_{12}\Delta_1 + W_{11}\Delta_2)^2 - (\omega^2 - \tilde{\in}_2^2)(W_{11}\Delta_1 + W_{12}\Delta_2)^2 \\ - 2W_{12}^2\gamma^2(\omega^2 + \tilde{\in}_1\tilde{\in}_2)\end{array}\right]} \quad \ldots(13)$$

On further simplification, one obtains

$$F_{11} = -\frac{1}{4\pi\alpha_1(\alpha_1^2 - \alpha_2^2)}\left[\frac{P+Q}{(\omega - \alpha_1)} + \frac{P-Q}{(\omega + \alpha_1)}\right] - \frac{1}{4\pi\alpha_2(\alpha_1^2 - \alpha_2^2)}\left[\frac{P_1+Q_1}{(\omega - \alpha_2)} + \frac{P_1-Q_1}{(\omega + \alpha_2)}\right] \quad \ldots(14)$$

Where

$$P = -\alpha_1 W_{12}\gamma\{(W_{11}\Delta_1 + W_{12}\Delta_2) - (W_{12}\Delta_1 + W_{11}\Delta_2)\}$$

$$Q = \alpha_1^2(W_{11}\Delta_1 + W_{12}\Delta_2) - \tilde{\in}_2^2(W_{11}\Delta_1 + W_{12}\Delta_2) - W_{12}\gamma\{(W_{11}\Delta_1 + W_{12}\Delta_2)\tilde{\in}_2 + (W_{12}\Delta_1 + W_{11}\Delta_2)\tilde{\in}_1\}$$

$$P_1 = \alpha_2 W_{12}\gamma\{(W_{11}\Delta_1 + W_{12}\Delta_2) - (W_{12}\Delta_1 + W_{11}\Delta_2)\}$$

$$Q_1 = -\alpha_2^2(W_{11}\Delta_1 + W_{12}\Delta_2) + \tilde{\in}_2^2(W_{11}\Delta_1 + W_{12}\Delta_2) + W_{12}\gamma\{(W_{11}\Delta_1 + W_{12}\Delta_2)\tilde{\in}_2 + (W_{12}\Delta_1 + W_{11}\Delta_2)\tilde{\in}_1\}$$

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

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

Correlation functions

Using the following relation[19-23]

$$\left\langle C_K^+ C_K \right\rangle = \frac{1}{2\pi}\int_{-\infty}^{\infty} I_G(\omega_N)\exp\{-i\omega_n(t - t')\}d\omega_n \quad \ldots(15)$$

Substituting t = t/ we get

$$\left\langle C_K^+ C_K \right\rangle = \frac{1}{2\pi}\int_{-\infty}^{\infty} I_G(\omega_N)d\omega_n \quad \ldots(16)$$

Where

$$I_G(\omega_n) = \frac{i}{e^{\beta\omega_n}+1}\left[G_{11}(\omega_n + i\in) - G_{11}(\omega_n - i\in)\right] \qquad \text{...(17)}$$

and employing the following identity

$$\lim_{\in\to 0}\left[\frac{1}{\omega + i\in - E_K} - \frac{1}{\omega - i\in - E_K}\right] = 2\pi i\,\delta(\omega - E_K) \qquad \text{...(18)}$$

We obtain the correlation function for the Green's function given by Eq. (12) as –

$$\left\langle C_K^{+}C_K \right\rangle = \left[\frac{1}{4\pi} + \frac{1}{4\pi\alpha_1\alpha_2^2(\alpha_1^2-\alpha_2^2)}\left\{Y\tanh\left(\frac{\beta\alpha_1}{2}\right) + \alpha_1\alpha_2 Y_1 W_{12}\gamma\tanh\left(\frac{\beta\alpha_2}{2}\right)\right\}\right] \qquad \text{...(19)}$$

where

$$\frac{Y}{4\pi\alpha_1\alpha_2^2(\alpha_1^2-\alpha_2^2)} = \frac{1}{4\pi}\left[\frac{\tilde{\in}_1}{\alpha_1} - \frac{W_{12}\gamma}{\alpha_1(\alpha_1^2-\alpha_2^2)}\tilde{\in}_1\tilde{\in}_2 - \frac{\alpha_1 W_{12}\gamma}{(\alpha_1^2-\alpha_2^2)}\right] \qquad \text{...(20)}$$

and

$$\frac{Y_1 W_{12}\gamma}{4\pi\alpha_2(\alpha_1^2-\alpha_2^2)} = \frac{W_{12}\gamma\left[\tilde{\in}_2^{\,2} + W'^2 + \tilde{\in}_1\tilde{\in}_2\right]}{4\pi\alpha_2(\alpha_1^2-\alpha_2^2)} \qquad \text{...(21)}$$

Similarly, we obtain the correlation function for the Green's function given by Eq. (14) as –

$$\left\langle C_K C_K \right\rangle = \frac{1}{4\pi(\alpha_1^2-\alpha_2^2)}\left[\begin{array}{l} \dfrac{W\alpha_1^2 - \left\{W\,\tilde{\in}_2^{\,2} + W_{12}\gamma\left(W\,\tilde{\in}_2 + W'\,\tilde{\in}_1\right)\right\}}{\alpha_1}\tanh\left(\dfrac{\beta\alpha_1}{2}\right) \\ -\dfrac{W\alpha_2^2 - \left\{W\,\tilde{\in}_2^{\,2} + W_{12}\gamma\left(W\,\tilde{\in}_2 + W'\,\tilde{\in}_1\right)\right\}}{\alpha_2}\tanh\left(\dfrac{\beta\alpha_2}{2}\right) \end{array}\right] \qquad \text{...(22)}$$

Where

$W' = W_{12}\,\Delta_1 + W_{11}\,\Delta_2$ ...(23)

$W = W_{11}\,\Delta_1 + W_{12}\,\Delta_2$ ...(24)

Physical properties

Superconducting order parameter

Superconducting order parameter (Δ) is given by –

$$\Delta = |g| \sum_{K} \langle C_K C_K \rangle \qquad \ldots(25)$$

Now using Eq. (22) we obtain

$$\Delta = |g| \sum_{K} \frac{1}{4\pi(\alpha_1^2 - \alpha_2^2)} \left[\frac{W\alpha_1^2 - \{W \tilde{\epsilon}_2^{\,2} + W_{12}\gamma(W \tilde{\epsilon}_2 + W' \tilde{\epsilon}_1)\}}{\alpha_1} \tanh\left(\frac{\beta\alpha_1}{2}\right) - \frac{W\alpha_2^2 - \{W \tilde{\epsilon}_2^{\,2} + W_{12}\gamma(W \tilde{\epsilon}_2 + W' \tilde{\epsilon}_1)\}}{\alpha_2} \tanh\left(\frac{\beta\alpha_2}{2}\right) \right]$$

$$\Delta = |g| \sum_{K} \left[\frac{W}{4\pi(\alpha_1^2 - \alpha_2^2)} \left\{ \alpha_1 \tanh\left(\frac{\beta\alpha_1}{2}\right) - \alpha_2 \tanh\left(\frac{\beta\alpha_2}{2}\right) \right\} - \frac{\{W \tilde{\epsilon}_2^{\,2} + W_{12}\gamma(W \tilde{\epsilon}_2 + W' \tilde{\epsilon}_1)\}}{4\pi(\alpha_1^2 - \alpha_2^2)} \left\{ \frac{1}{\alpha_1} \tanh\left(\frac{\beta\alpha_1}{2}\right) - \frac{1}{\alpha_2} \tanh\left(\frac{\beta\alpha_2}{2}\right) \right\} \right] \qquad \ldots(26)$$

Applying identity,

$$\sum_{K} = 2N(0) \int_0^{\hbar\omega_D} d\,\epsilon_\alpha \qquad \ldots(27)$$

We get

$$\Delta = 2N(0)|g| \int_0^{\hbar\omega_D} \left[\frac{W}{4\pi(\alpha_1^2 - \alpha_2^2)} \left\{ \alpha_1 \tanh\left(\frac{\beta\alpha_1}{2}\right) - \alpha_2 \tanh\left(\frac{\beta\alpha_2}{2}\right) \right\} - \frac{\{W \tilde{\epsilon}_2^{\,2} + W_{12}\gamma(W \tilde{\epsilon}_2 + W' \tilde{\epsilon}_1)\}}{4\pi(\alpha_1^2 - \alpha_2^2)} \left\{ \frac{1}{\alpha_1} \tanh\left(\frac{\beta\alpha_1}{2}\right) - \frac{1}{\alpha_2} \tanh\left(\frac{\beta\alpha_2}{2}\right) \right\} \right] d\,\epsilon_\alpha \qquad \ldots(28)$$

Where W, W', α_1 and α_2 are defined in previous section and

$$\alpha_1^2 - \alpha_2^2 = \tilde{\epsilon}_1^2 - \tilde{\epsilon}_2^2 + (W_{11}\Delta_1 + W_{12}\Delta_2)^2 - (W_{12}\Delta_1 + W_{11}\Delta_2)^2 - 2W_{12}^2\gamma^2$$

$$\tilde{\epsilon}_1 = \epsilon_1 - \mu - \frac{W_{11}}{2}$$

$$\tilde{\epsilon}_2 = \epsilon_2 - \mu - \frac{W_{11}}{2}$$

Case 1:

For Δ_1, applying $\tilde{\epsilon}_2 = 0$ and $\Delta_2 = 0$ in Eq. (28), we get,

$$\Delta_1 = 2N(0)|g| \int_0^{\hbar\omega_D} \left[\begin{array}{l} \dfrac{W_{11}\Delta_1}{4\pi\left(\alpha_1^2-\alpha_2^2\right)} \left\{ \alpha_1 \tanh\left(\dfrac{\beta\alpha_1}{2}\right) - \alpha_2 \tanh\left(\dfrac{\beta\alpha_2}{2}\right) \right\} \\ - \dfrac{W_{12}\Delta_1 \tilde{\in}_1 W_{12}\gamma}{4\pi\left(\alpha_1^2-\alpha_2^2\right)} \left\{ \dfrac{1}{\alpha_1} \tanh\left(\dfrac{\beta\alpha_1}{2}\right) - \dfrac{1}{\alpha_2} \tanh\left(\dfrac{\beta\alpha_2}{2}\right) \right\} \end{array} \right] d \in_1 \quad \ldots(29)$$

$$\begin{aligned} \frac{1}{|g|N(0)} = {} & \frac{W_{11}}{2\pi} \int_0^{\hbar\omega_D} \frac{\sqrt{\left(\in_1 - \frac{W_{11}}{2}\right)^2 + W_{11}^2\Delta_1^2}}{\left\{\left(\in_1 - \frac{W_{11}}{2}\right)^2 + \left(W_{11}^2 - W_{12}^2\right)\Delta_1^2 - 2W_{12}^2\gamma^2\right\}} \tanh \frac{1}{2k_BT} \sqrt{\left(\in_1 - \frac{W_{11}}{2}\right)^2 + W_{11}^2\Delta_1^2}\, d \in_1 \\ & - \frac{W_{12}^2\gamma}{2\pi} \int_0^{\hbar\omega_D} \frac{\in_1 - \frac{W_{11}}{2}}{\left\{\left(\in_1 - \frac{W_{11}}{2}\right)^2 + \left(W_{11}^2 - W_{12}^2\right)\Delta_1^2 - 2W_{12}^2\gamma^2\right\}\sqrt{\left(\in_1 - \frac{W_{11}}{2}\right)^2 + W_{11}^2\Delta_1^2}} \tanh \frac{1}{2k_BT} \sqrt{\left(\in_1 - \frac{W_{11}}{2}\right)^2 + W_{11}^2\Delta_1^2}\, d \in_1 \\ & - \frac{W_{11}W_{12}}{2\pi} \cdot \frac{\sqrt{\Delta_1^2 + 2\gamma^2}}{\sqrt{\left(W_{11}^2 - W_{12}^2\right)\Delta_1^2 - 2W_{12}^2\gamma^2}} \tanh \frac{W_{12}}{2k_BT}\sqrt{\Delta_1^2 + 2\gamma^2} \left[\tan^{-1}\left(\frac{\hbar\omega_D - \frac{W_{11}}{2}}{\sqrt{\left(W_{11}^2 - W_{12}^2\right)\Delta_1^2 - 2W_{12}^2\gamma^2}} \right) - \tan^{-1}\left(\frac{-\frac{W_{11}}{2}}{\sqrt{\left(W_{11}^2 - W_{12}^2\right)\Delta_1^2 - 2W_{12}^2\gamma^2}} \right) \right] \\ & + \frac{W_{12}\gamma}{4\pi} \cdot \frac{1}{\sqrt{\Delta_1^2 + 2\gamma^2}} \tanh \frac{W_{12}}{2k_BT}\sqrt{\Delta_1^2 + 2\gamma^2} \left[\log_e \frac{\left(\hbar\omega_D - \frac{W_{11}}{2}\right)^2 + \left(W_{11}^2 - W_{12}^2\right)\Delta_1^2 - 2W_{12}^2\gamma^2}{\frac{W_{11}^2}{4} + \left(W_{11}^2 - W_{12}^2\right)\Delta_1^2 - 2W_{12}^2\gamma^2} \right] \quad \ldots(30) \end{aligned}$$

Case 2:

For Δ_2, applying $\tilde{\in}_1 = 0$ and $\Delta_1 = 0$ in Eq. (28), we get

$$\Delta_2 = 2N(0)|g| \int_0^{\hbar\omega_D} \left[\frac{W_{12}\Delta_2}{4\pi\left(\alpha_1^2-\alpha_2^2\right)} \left\{ \alpha_1 \tanh\left(\frac{\beta\alpha_1}{2}\right) - \alpha_2 \tanh\left(\frac{\beta\alpha_2}{2}\right) \right\} - \frac{\left\{W_{12}\Delta_2 \tilde{\in}_2^{\,2} + W_{12}^{\,2}\Delta_2\gamma\, \tilde{\in}_2\right\}}{4\pi\left(\alpha_1^2-\alpha_2^2\right)} \left\{ \frac{1}{\alpha_1} \tanh\left(\frac{\beta\alpha_1}{2}\right) - \frac{1}{\alpha_2} \tanh\left(\frac{\beta\alpha_2}{2}\right) \right\} \right] d \in_2 \quad \ldots(31)$$

$$\begin{aligned} \frac{1}{|g|N(0)} = {} & \frac{1}{2\pi\Delta_2} \int_0^{\hbar\omega_D} \frac{\left\{\left(\in_2 - \frac{W_{11}}{2}\right)^2 + W_{12}\gamma\left(\in_2 - \frac{W_{11}}{2}\right) - W_{12}^2\Delta_2^2\right\}}{\left\{\left(\in_2 - \frac{W_{11}}{2}\right)^2 + \left(W_{11}^2 - W_{12}^2\right)\Delta_2^2 + 2W_{12}^2\gamma^2\right\}} \tanh \frac{\beta W_{12}\Delta_2}{2}\, d \in_2 \\ & - \int_0^{\hbar\omega_D} \frac{\left\{W_{12}^2\gamma\left(\in_2 - \frac{W_{11}}{2}\right)\right\} - W_{12}W_{11}^2\Delta_2^2 - 2W_{12}^3\gamma^2}{2\pi\left\{\left(\in_2 - \frac{W_{11}}{2}\right)^2 + \left(W_{11}^2 - W_{12}^2\right)\Delta_2^2 + 2W_{12}^2\gamma^2\right\}\sqrt{\left(\in_2 - \frac{W_{11}}{2}\right)^2 + W_{11}^2\Delta_2^2 + 2W_{12}^2\gamma^2}}. \quad \ldots(32) \\ & \tanh \frac{\beta}{2}\sqrt{\left(\in_2 - \frac{W_{11}}{2}\right)^2 + W_{11}^2\Delta_2^2 + 2W_{12}^2\gamma^2}\,.d \in_2 \end{aligned}$$

We have solved Eqs. (30) and (32) numerically with parameters shown in Table 1.

Table 1: Values of various parameters for magnesium diboride (MgB_2) system

Parameter	Value	Reference
Superconducting transition temperature	39 K	1
Phonon energy (ϵ_1)	0.06 eV	25
Phonon energy (ϵ_2)	0.05 eV	25
Density of states at the Fermi surface	3.093 / eV.atom	25
Pairing interaction $W_{11} = W_{22}$ intra-band	0.3 eV.cell	13
Pairing interaction $W_{12} = W_{21}$ inter-band	0.0001 eV.cell	13
No. of atoms per unit volume	$5 \times 10^{28} / m^3$	31
Cell parameter	a = 3.086 Å b = 3.524 Å	26
Boltzmann constant	1.38×10^{-23} J/K	-
Mass of electron	9.1×10^{-31} Kg	-

Electronic specific heat

The electronic specific heat per atom of a superconductor is given by[3,19-24] –

$$C_{es} = \frac{\partial}{\partial T}\left[\frac{1}{N}\sum_K 2 \in_K \left\langle C_K^{+} C_K \right\rangle\right] \qquad \ldots(33)$$

Using Eq. (19) and choosing summation over K into an integration using

$$\sum_K = N(0)\int d \in_K \qquad \ldots(34)$$

One obtain

$$C_{es} = \frac{2N(0)}{N}\int_0^{\hbar\omega_D} \frac{\in_K}{8\pi k_B T^2(\alpha_1^2 - \alpha_2^2)}\left[\begin{array}{l}\left\{(\alpha_1^2 - \alpha_2^2)\tilde{\in}_1 - W_{12}\gamma(\alpha_1^2 + \tilde{\in}_1\tilde{\in}_2)\right\}\sec h^2 \dfrac{\beta\alpha_1}{2} + \\ W_{12}\gamma(\alpha_2^2 + \tilde{\in}_1\tilde{\in}_2)\sec h^2 \dfrac{\beta\alpha_2}{2}\end{array}\right] d \in_K \qquad \ldots(35)$$

Case 1:

For C_{es}^{1}, applying $\tilde{\in}_2 = 0$ and $\Delta_2 = 0$ in Eq. (35) we get,

$$C_{es}^{1} = \frac{N(0)}{N}\frac{1}{4\pi k_B T^2}\left[\begin{array}{l} \int_0^{\hbar\omega_D} \in_1 \left(\in_1 - \frac{W_{11}}{2}\right)\sec h^2 \frac{\beta}{2}\sqrt{\left(\in_1 - \frac{W_{11}}{2}\right)^2 + W_{11}{}^2\Delta_1{}^2}\, d\in_1 \\ -W_{12}\gamma\int_0^{\hbar\omega_D} \frac{\in_1\left(\left(\in_1 - \frac{W_{11}}{2}\right)^2 + W_{11}{}^2\Delta_1{}^2\right)}{\left(\left(\in_1 - \frac{W_{11}}{2}\right)^2 + \left(W_{11}{}^2 - W_{12}{}^2\right)\Delta_1{}^2 - 2W_{12}{}^2\gamma^2\right)}\sec h^2 \frac{\beta}{2}\sqrt{\left(\in_1 - \frac{W_{11}}{2}\right)^2 + W_{11}{}^2\Delta_1{}^2}\, d\in_1 \\ +W_{12}{}^3\gamma\left(\Delta_1{}^2 + 2\gamma^2\right)\sec h^2 \frac{\beta}{2} W_{12}\sqrt{\Delta_1{}^2 + 2\gamma^2}\int_0^{\hbar\omega_D} \frac{\in_1}{\left(\left(\in_1 - \frac{W_{11}}{2}\right)^2 + \left(W_{11}{}^2 - W_{12}{}^2\right)\Delta_1{}^2 - 2W_{12}{}^2\gamma^2\right)}\, d\in_1 \end{array}\right] \quad \ldots(36)$$

Case 2:

For C_{es}^{2}, applying $\tilde{\in}_1 = 0$ and $\Delta_1 = 0$ in Eq. (35), we get

$$C_{es}^{2} = \frac{N(0)}{N}\frac{W_{12}\gamma}{4\pi k_B T^2}\left[\begin{array}{l} W_{12}^2\Delta_2{}^2\,\mathrm{sech}^2\frac{W_{12}\Delta_2}{2k_B T}\int_0^{\hbar\omega_D}\frac{\in_2}{\left(\left(\in_2 - \frac{W_{11}}{2}\right)^2 + \left(W_{11}^2 - W_{12}^2\right)\Delta_2{}^2 + 2W_{12}^2\gamma^2\right)}\, d\in_2 \\ -\int_0^{\hbar\omega_D}\frac{\in_2\left(\left(\in_2 - \frac{W_{11}}{2}\right)^2 + W_{11}^2\Delta_2{}^2 + 2W_{12}{}^2\gamma^2\right)}{\left(\left(\in_2 - \frac{W_{11}}{2}\right)^2 + \left(W_{11}^2 - W_{12}^2\right)\Delta_2{}^2 + 2W_{12}^2\gamma^2\right)}\mathrm{sech}^2\frac{\beta}{2}\sqrt{\left(\left(\in_2 - \frac{W_{11}}{2}\right)^2 + W_{11}^2\Delta_2{}^2 + 2W_{12}^2\gamma^2\right)}\, d\in_2 \end{array}\right] \quad \ldots(37)$$

We have solved Eqs. (36) and (37) numerically with parameters shown in Table 1.

Numerical calculations

We now evaluate numerically Δ and C_{es} using the parameters given in Table 1 for MgB_2.

Superconducting order parameter (Δ)

For the study of superconducting order parameter for MgB_2 system within two band model, one finds the following situations:

Superconducting order parameter 1 ($\Delta 1$)

Choosing

$W_{11} = W_{22} = 0.3$ eV. cell $= 9.6 \times 10^{-21}$ J

$W_{12} = W_{21} = z$ eV.cell $= z \times 32 \times 10^{-21}$J $\gamma = (-)\ 0.01753$

$\epsilon_1 = 0.06$ y eV $= 9.6 \times 10^{-21}$ y J $k_B = 1.38 \times 10^{-23}$ J/K

$\hbar\omega_D = 0.06$eV $\Delta_1 = x$

Now putting in Eq. (30) and solving, we obtain

$$\frac{1}{|g|N(0)} = 1.528X10^{-21}\int_{y=0}^{y=1}\frac{\sqrt{(y-0.5)^2+x^2}}{\left[(y-0.5)^2+(1-11.11z^2)x^2-0.00683z^2\right]}\tanh\frac{347.82}{T}\sqrt{(y-0.5)^2+x^2}\,dy \quad \ldots(38)$$

$$+0.2978X10^{-21}z^2\int_{y=0}^{y=1}\frac{(y-0.5)}{\sqrt{(y-0.5)^2+x^2}\left[\left[(y-0.5)^2+(1-11.11z^2)x^2-0.00683z^2\right]\right]}\tanh\frac{347.82}{T}\sqrt{(y-0.5)^2+x^2}\,dy$$

$$-5.096X10^{-21}z\frac{\sqrt{x^2+0.000614}}{\sqrt{(1-11.11z^2)x^2-0.00683z^2}}\tanh\frac{11.594}{T}z\sqrt{x^2+0.000614}\left[\begin{array}{l}\tan^{-1}\left(\dfrac{1}{2\sqrt{(1-11.11z^2)x^2-0.00683z^2}}\right)\\ -\tan^{-1}\left(-\dfrac{1}{2\sqrt{(1-11.11z^2)x^2-0.00683z^2}}\right)\end{array}\right]$$

Superconducting order parameter 2 (Δ_2)

Choosing

$W_{11} = W_{22} = 0.3$ eV.cell $= 9.6 \times 10^{-21}$J

$W_{12} = W_{21} = z$ eV.cell $= z \times 32 \times 10^{-21}$J $\gamma = (-)\ 0.01753$

$\epsilon_2 = 0.05$ y eV $= 8 \times 10^{-21}$ y J $k_B = 1.38 \times 10^{-23}$ J/K

$\hbar\omega_D = 0.05$ eV $\Delta_2 = x$

Now putting in Eq. (32) and solving, we obtain

$$\frac{1}{|g|N(0)} = 1.273X10^{-21}/x\ \tanh\frac{1159.4}{T}zx\left[\begin{array}{l}1-0.03506z\log_e\dfrac{10.24+x^2(92.16-1024z^2)+0.629z^2}{23.04+x^2(92.16-1024z^2)+0.629z^2}\\ -1.2\dfrac{x^2+0.00682z^2}{\sqrt{x^2(1-11.11z^2)+0.00682z^2}}\left\{\begin{array}{l}\tan^{-1}\left(\dfrac{1}{3\sqrt{(1-11.11z^2)x^2-0.00682z^2}}\right)\\ -\tan^{-1}\left(-\dfrac{1}{2\sqrt{(1-11.11z^2)x^2-0.00682z^2}}\right)\end{array}\right\}\end{array}\right]$$

$$+0.3573X10^{-21}z^2 *$$

$$\int_{y=0}^{y=1}\frac{(y-0.6)}{\sqrt{(y-0.6)^2+1.44x^2+0.00983z^2}\left[(y-0.6)^2+1.44(1-11.11z^2)x^2+0.00983z^2\right]}\tanh\frac{289.85}{T}\sqrt{(y-0.6)^2+1.44x^2+0.00983z^2}\,dy$$

$$+0.7643X10^{-21}z\left(x^2+0.00682z^2\right)*$$

$$\int_{y=0}^{y=1}\frac{1}{\sqrt{(y-0.6)^2+1.44x^2+0.00983z^2}\left[(y-0.6)^2+1.44(1-11.11z^2)x^2+0.00983z^2\right]}\tanh\frac{289.85}{T}\sqrt{(y-0.6)^2+1.44x^2+0.00983z^2}\,dy \quad \ldots(39)$$

Solving numerically Eq. (38) and (39), we obtain variations of superconducting order parameters (Δ_1, Δ_2 and Δ) with temperature as shown in Figs. 1, 2 and 3, respectively for W_{12} = 0.0001 eV. cell (Tables 2, 3 and 4).

Table 2: Superconducting order parameter (Δ_1) for magnesium diboride (MgB_2) system

Temp. (K)	Δ_1 (Theoretical) (meV)	Δ_1 (Experimental) (meV)
5	0.6241	2.90
10	0.6236	2.86
15	0.6164	2.82
20	0.5941	2.70
25	0.5487	2.20
30	0.4702	1.70
32	0.4251	1.35
35	0.3331	0.88
36	0.2922	0.72
37	0.2414	0.45
38	0.1725	0.20
39	0.0056	0.00

Table 3: Superconducting order parameter (Δ_2) for magnesium diboride (MgB_2) system

Temp. (K)	Δ_2 (Theoretical) (meV)	Δ_2 (Experimental) (meV)
5	6.1169	7.20
10	5.7075	7.16
15	4.5750	6.93
20	2.8313	6.40
25	1.8225	5.70
30	1.0531	4.15
32	0.7638	3.43
35	0.3116	2.30
36	0.1971	1.90
37	0.1142	1.20
38	0.0513	0.60
39	0.0006	0.00

Table 4: Superconducting order parameter ($\Delta = \Delta_1 + \Delta_2$) for magnesium diboride (MgB_2) system

Temp. (K)	$\Delta = \Delta_1 + \Delta_2$ (Theoretical) (meV)	$\Delta = \Delta_1 + \Delta_2$ (Experimental) (meV)
5	6.7410	10.10
10	6.3311	10.02
15	5.1914	9.75
20	3.4254	9.10
25	2.3712	7.91
30	1.5233	5.85
32	1.1889	4.78
35	0.6447	3.18
36	0.4893	2.65
37	0.3556	1.65
38	0.2238	0.80
39	0.00620	0.00

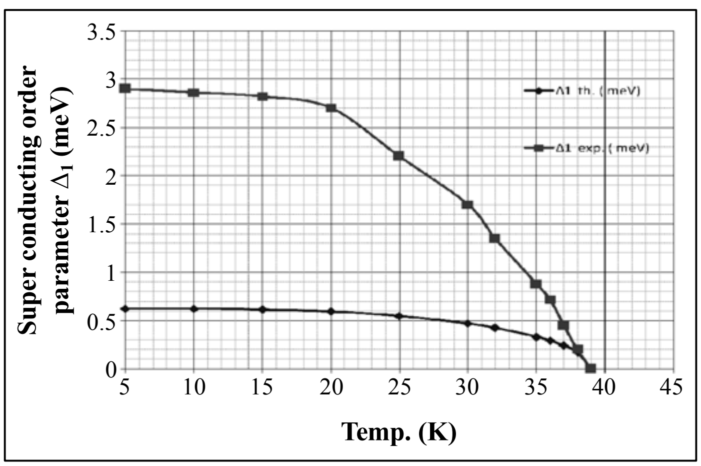

Fig. 1: Variations of superconducting order parameter (Δ_1) with temperature for magnesium diboride (MgB_2) system

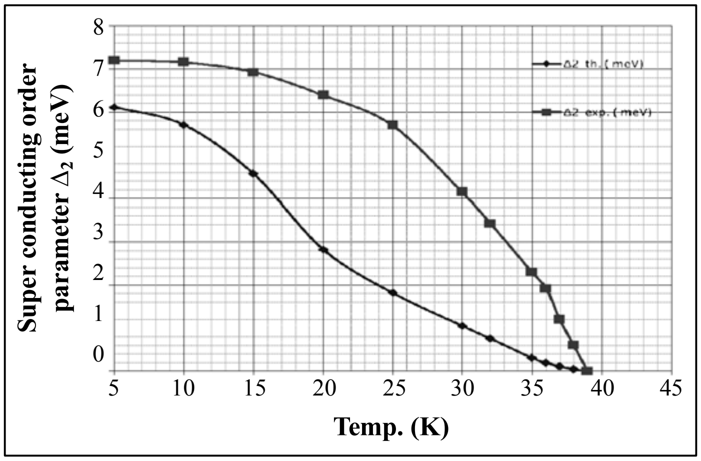

Fig. 2: Variations of superconducting order parameter (Δ_2) with temperature for magnesium diboride (MgB_2) system

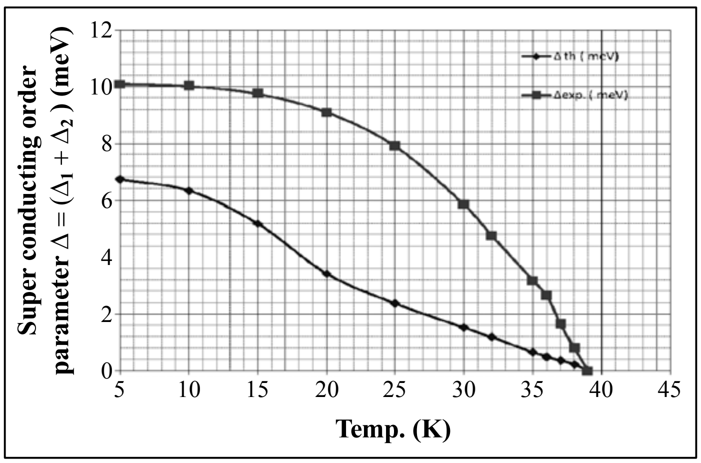

Fig. 3: Variations of superconducting order parameter ($\Delta = \Delta_1 + \Delta_2$) with temperature for magnesium diboride (MgB_2) system.

Electronic specific heat

Substituting following values in Eq. (36) for C^1_{es}

$W_{11} = W_{22} = 0.3$ eV. cell $= 9.6 \times 10^{-21}$ J

$W_{12} = W_{21} = z$ eV. cell $= z \times 32 \times 10^{-21}$ J $\qquad \gamma = (-)\ 0.01753$

$\epsilon_1 = 0.06\ y$ eV $= 9.6 \times 10^{-21}\ y$ J $\qquad k_B = 1.38 \times 10^{-23}$ J/K

$\hbar\omega_D = 0.06$ eV $\Delta_1 = x$

N (0) = 3.093 / eV.atom N = 5 x $10^{28}/m^3$

We obtain

$$C_{es}^{1} = \frac{32.8\times10^{-49}}{T^{2}}\left[1.54\int_{y=0}^{y=1}(y-0.5)\sec h^{2}\frac{347.82}{T}\left\{\sqrt{(y-0.5)^{2}+x^{2}}\right\}dy + 0.09z\int_{y=0}^{y=1}\frac{y\left\{(y-0.5)^{2}+x^{2}\right\}\sec h^{2}\frac{347.82}{T}\left\{\sqrt{(y-0.5)^{2}+x^{2}}\right\}dy}{\left[(y-0.5)^{2}+\left(1-11.11z^{2}\right)x^{2}-0.00683z^{2}\right]} - z^{3}\left(x^{2}+0.000614\right)\sec h^{2}\frac{1159.4}{T}z\left(x^{2}+0.000614\right)\int_{y=0}^{y=1}\frac{ydy}{\left[(y-0.5)^{2}+\left(1-11.11z^{2}\right)x^{2}-0.00683z^{2}\right]}\right] \quad (40)$$

Substituting following values in Eq. (37) for C_{es}^{2}

$W_{11} = W_{22} = 0.3$ eV.cell = 9.6 x 10^{-21}J

$W_{12} = W_{21} = z$ eV.cell =z x 32 x 10^{-21}J γ = (-) 0.01753

$\epsilon_2 = 0.05$ y eV = 8 x 10^{-21} y J $k_B = 1.38$ x 10^{-23} J/K

$\hbar\omega_D = 0.05$eV $\Delta_2 = x$

N (0) = 3.093 / eV.atom N = 5 x $10^{28}/m^3$

We obtain

$$C_{es}^{2} = \frac{2.05\times10^{-49}}{T^{2}}\left[-16z^{2}x^{2}\sec h^{2}\frac{1159.4}{T}zx\int_{y=0}^{y=1}\frac{ydy}{(y-0.6)^{2}+1.44\left(1-11.11z^{2}\right)x^{2}-0.00683z^{2}} + \int_{y=0}^{y=1}\frac{y\left\{(y-0.6)^{2}+1.44x^{2}-0.00683z^{2}\right\}\sec h^{2}\frac{289.85}{T}\sqrt{(y-0.6)^{2}+1.44x^{2}-0.00683z^{2}}\,dy}{(y-0.6)^{2}+1.44\left(1-11.11z^{2}\right)x^{2}-0.00683z^{2}}\right] \quad (41)$$

Solving numerically Eq. (40) and (41), we obtain variations of C_{es} with temperature for W_{12} = 0.0001 eV. cell as shown in Fig. 4 (Table 5).

Table 5: Electronic specific heat (Ces) for magnesium diboride (MgB_2) system

Temp. (K)	C_{es} (Theoretical) = C^1_{es}+ C^2_{es} in J/mole-K	C_{es} (Experimental) in J/mole-K
5	0.00006	1.9
10	0.2792	10.1
15	3.6511	29.1
20	12.8391	45.3
25	27.9675	64.0
30	48.4162	91.8
32	57.9393	99.2
35	73.5297	113.9
36	79.0362	112.1
37	84.7204	110.7
38	90.5759	105.3
39	96.5675	101.2

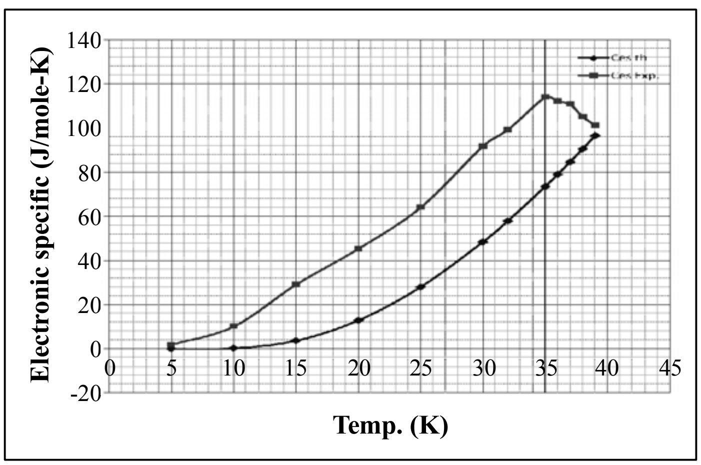

Fig. 4: Variations of electronic specific heat C_{es} with temperature for magnesium diboride (MgB_2) system

CONCLUSION

In the previous sections, we have presented the study of superconductivity in magnesium diboride based on multi band Hamiltonian with intra- and inter-band pair transfer interactions. Following the Green's function technique and equation of motion method, we have obtained the expressions for superconducting order parameters Δ_1, Δ_2 and $\Delta = \Delta_1 + \Delta_2$ as well as for electronic specific heat C_{es}.

Making use of various parameters given in Table 1 for the system MgB_2, we have studied the above cited physical properties and compared our results with the available experimental data. Our results and conclusions are as follows:

(i) The transition temperature for our system MgB_2 is found to be 39 K[1].

(ii) The temperature dependent two superconducting order parameter Δ_1, Δ_2 and $\Delta = \Delta_1 + \Delta_2$ with temperature for value of matrix element of inter-band interaction $W_{12} = 0.0001$ eV.cell have been studied. The two gap structure is in agreement with experimental observations[27].

(iii) The variation of electronic specific heat (C_{es}) with temperature obtained from our model is studied for value of matrix element of inter-band interaction $W_{12}= 0.0001$ eV.cell.

The results obtained are in good agreement with experimental results[28].

Our model shows reasonable agreement with available experimental data. Two band mechanisms emerges as a strong contender for an acceptable model for MgB_2 – inter metallic binary compounds. The efforts to understand the pairing mechanism in MgB_2 and other similar systems should be continued, for such efforts has to go hand-in-hand with enhancing future prospects for new superconducting materials and novel applications.[29-36]

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