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

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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 ($\Delta$) 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

Magnesium 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 compounds2.

Magnesium diboride is receiving attention due to exceptionally high values of critical temperature and critical field. This material may be suitable contender to replace Nb3Sn or NbTi as the choice for practical large scale application in the range of 20-30 K operating with cryogenic refrigerators.
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 $\sigma$ band orbital and the second one is the broader band built up mainly of $\pi$ 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 $\sigma$ and $\pi$ 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$^{13}$.

$$
H = \sum_{als} \varepsilon_\alpha(l) a_{\alpha l s}^+ a_{\alpha l s} - \frac{1}{V} \sum_{\alpha\alpha'} \sum_{l m} W_{\alpha\alpha'}(l, m) \left( a_{\alpha l}^+ a_{\alpha l} - a_{\alpha' m}^+ a_{\alpha' m} - \delta_{\alpha\alpha'} \right) \ldots (1)
$$

Where $\varepsilon_\alpha = \varepsilon_a - \mu$ is the electron energy in the bands $\alpha = 1, 2$; $\mu$ 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 –


\[ H = H_{11} + H_{22} + H_{12} + H_{21} \]  
\[ \ldots(2) \]

where

\[ H_{11} = \sum_{ls} \epsilon_p (l) a_{ls}^+ a_{ls} - \frac{1}{V} \sum_{lm} W_{11} (lm) a_{l}^+ a_{l}^+ 1 - l \downarrow 1 - m \downarrow a_{1m} \uparrow \]

\[ H_{22} = \sum_{ls} \epsilon_p (l) a_{2ls}^+ a_{2ls} - \frac{1}{V} \sum_{lm} W_{22} (lm) a_{2l}^+ a_{2l}^+ 2 - l \downarrow 2 - m \downarrow a_{2m} \uparrow \]

\[ H_{12} = \sum_{ls} \epsilon_p (l) a_{1ls}^+ a_{1ls} - \frac{1}{V} \sum_{lm} W_{12} (lm) a_{l}^+ a_{l}^+ 1 - l \downarrow 2 - m \downarrow a_{2m} \uparrow \]

\[ H_{21} = \sum_{ls} \epsilon_p (l) a_{2ls}^+ a_{2ls} - \frac{1}{V} \sum_{lm} W_{21} (lm) a_{2l}^+ a_{2l}^+ 2 - l \downarrow 1 - m \downarrow a_{1m} \uparrow \]  
\[ \ldots(3) \]

On solving, one obtain

\[ [a_{1k}^+, H] = \epsilon_p (k) a_{1k}^+ - \frac{1}{V} \sum_m W_{11} (k,m) a_{1-k-k}^+ a_{1-m}^+ a_{1m}^+ \]

\[ \ldots(4) \]

\[ [a_{2k}^+, H] = \epsilon_p (k) a_{2k}^+ - \frac{1}{V} \sum_m W_{22} (k,m) a_{2-k-k}^+ a_{2-m}^+ a_{2m}^+ \]

\[ \ldots(5) \]

\[ [a_{1-k}^+, H] = - \epsilon_p (-k) a_{1-k}^+ - \frac{1}{V} \sum_l W_{11} (l,k) a_{1-l-l}^+ a_{1-k}^+ \]

\[ \ldots(6) \]

\[ [a_{2-k}^+, H] = - \epsilon_p (-k) a_{2-k}^+ - \frac{1}{V} \sum_l W_{22} (l,k) a_{2-l-l}^+ a_{2-k}^+ \]

\[ \ldots(7) \]

**Green’s functions**

In order to study the physical properties, we define following normal & anomalous Green’s functions as follows\textsuperscript{14-24}:

\[ G_{11} (l,k,\uparrow) = \langle \langle a_{lk}^+ | a_{lk}^+ \rangle \rangle \]

\[ G_{22} (l,k,\uparrow) = \langle \langle a_{2k}^+ | a_{2k}^+ \rangle \rangle \]

\[ G_{21} (l,k,\uparrow) = \langle \langle a_{2k}^+ | a_{lk}^+ \rangle \rangle \]
\[ G_{12}(l, 2, k, \uparrow) = \left\langle a_{1k}^\uparrow | a_{2k}^\uparrow \right\rangle \]

\[ F_{11}(l, k, \uparrow) = \left\langle a_{1k}^+ \downarrow | a_{l1k}^\uparrow \right\rangle \]

\[ F_{12}(l, 2, k, \uparrow) = \left\langle a_{1k}^+ \downarrow | a_{2k}^\uparrow \right\rangle \]

\[ F_{21}(2, l, k, \uparrow) = \left\langle a_{2k}^+ \downarrow | a_{1k}^\uparrow \right\rangle \]

\[ F_{22}(2, k, \uparrow) = \left\langle a_{2k}^+ \downarrow | a_{2k}^\uparrow \right\rangle \]

…(8)

On solving, one get

\[
\begin{align*}
[\omega - \bar{\varepsilon}_1 (k)] G_{11} &= 1 - W_{12} \gamma_{12} G_{21} - \left[ W_{11} \Delta_{11} + W_{12} \Delta_{22} \right] F_{11} \\
[\omega - \bar{\varepsilon}_2 (k)] G_{22} &= 1 - W_{12} \gamma_{21} G_{12} - \left[ W_{12} \Delta_{11} + W_{22} \Delta_{22} \right] F_{22} \\
[\omega - \bar{\varepsilon}_2 (k)] G_{21} &= 1 - W_{12} \gamma_{21} G_{11} - \left[ W_{12} \Delta_{11} + W_{22} \Delta_{22} \right] F_{21} \\
[\omega - \bar{\varepsilon}_1 (k)] G_{12} &= 1 - W_{12} \gamma_{12} G_{22} - \left[ W_{11} \Delta_{11} + W_{12} \Delta_{22} \right] F_{12} \\
[\omega + \bar{\varepsilon}_1 (-k)] F_{11} &= W_{21} \gamma_{21} F_{21} - \left[ W_{11} \Delta_{11}^+ + W_{21} \Delta_{22}^+ \right] G_{11} \\
[\omega + \bar{\varepsilon}_2 (-k)] F_{22} &= W_{12} \gamma_{12} F_{12} - \left[ W_{12} \Delta_{11}^+ + W_{22} \Delta_{22}^+ \right] G_{22} \\
[\omega + \bar{\varepsilon}_2 (-k)] F_{21} &= W_{12} \gamma_{21} F_{11} - \left[ W_{12} \Delta_{11}^+ + W_{22} \Delta_{22}^+ \right] G_{21} \\
[\omega + \bar{\varepsilon}_1 (-k)] F_{12} &= W_{21} \gamma_{21} F_{22} - \left[ W_{11} \Delta_{11}^+ + W_{21} \Delta_{22}^+ \right] G_{12}
\end{align*}
\]

…(9)

Where

\[ \bar{\varepsilon}_1 (k) = \bar{\varepsilon}_1 (k) - W_{1} n_{1-k} \]

\[ n_{1-k} = \frac{1}{V} \left\langle a_{1-k}^- a_{1-k}^- \right\rangle \]

\[ \bar{\varepsilon}_2 (k) = \bar{\varepsilon}_2 (k) - W_{2} n_{2-k} \]

\[ n_{2-k} = \frac{1}{V} \left\langle a_{2-k}^+ a_{2-k}^+ \right\rangle \]
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

\[ W_{12} = W_{21} \]
\[ W_{11} = W_{22} \]
\[ \gamma_{12} = \gamma_{21} = \gamma \]
\[ \Delta_{11} = \Delta_{11}^+ = \Delta_1 \text{ and } \Delta_{22} = \Delta_{22}^+ = \Delta_2 \]

\[ G_{11} = \frac{1}{2\pi(i - \bar{\varepsilon}_2)(\omega - \bar{\varepsilon}_1)} \left[ \frac{X + Y}{(\omega - \alpha_1)} + \frac{X - Y}{(\omega + \alpha_1)} \right] + \frac{W_{12}}{4\pi\alpha_2(\alpha_1^2 - \alpha_2^2)} \left[ \frac{X_1 + Y_1}{(\omega - \alpha_2)} + \frac{X_1 - Y_1}{(\omega + \alpha_2)} \right] \]

On further simplification, one obtain

\[ G_{11} = \frac{1}{2\pi(i - \bar{\varepsilon}_2)(\omega - \bar{\varepsilon}_1)} \left[ \frac{X + Y}{(\omega - \alpha_1)} + \frac{X - Y}{(\omega + \alpha_1)} \right] + \frac{W_{12}}{4\pi\alpha_2(\alpha_1^2 - \alpha_2^2)} \left[ \frac{X_1 + Y_1}{(\omega - \alpha_2)} + \frac{X_1 - Y_1}{(\omega + \alpha_2)} \right] \]

Where

\[ X = \alpha_1^2 \bar{\varepsilon}_1^2 - \alpha_1^2 \bar{\varepsilon}_2^2 - \alpha_2^2 \bar{\varepsilon}_1^2 W_{12} \bar{\varepsilon}_1 - \alpha_1^2 \alpha_2^2 W_{12} \bar{\varepsilon}_1 \bar{\varepsilon}_2 + \alpha_1^2 \alpha_2^2 W_{12}^2 \bar{\varepsilon}_1^2 \]
\[ Y = \left( \alpha_1^2 - \alpha_2^2 \right) \bar{\varepsilon}_1 \bar{\varepsilon}_2 + \left( W_{12} \Delta_1 + W_{11} \Delta_2 \right)^2 - \alpha_1^2 \bar{\varepsilon}_1 \bar{\varepsilon}_2 W_{12} \bar{\varepsilon}_1 + \alpha_1^2 \bar{\varepsilon}_2 W_{12} \bar{\varepsilon}_2 \bar{\varepsilon}_1 \bar{\varepsilon}_2 W_{12}^2 \bar{\varepsilon}_1^2 - 2\alpha_1^2 W_{12}^3 \bar{\varepsilon}_1^2 \bar{\varepsilon}_2^2 \]
\[ + 2\alpha_1^2 \bar{\varepsilon}_1 \bar{\varepsilon}_2 W_{12} \bar{\varepsilon}_1^2 - \alpha_1^2 \bar{\varepsilon}_1^2 W_{12} \bar{\varepsilon}_2 - \alpha_1^2 \bar{\varepsilon}_2 W_{12} \bar{\varepsilon}_1 \bar{\varepsilon}_2 \bar{\varepsilon}_1 W_{12}^2 \bar{\varepsilon}_1^2 - 2\alpha_1^2 W_{12}^3 \bar{\varepsilon}_1^2 \bar{\varepsilon}_2^2 \]
\[ X_1 = \alpha_1^2 \left( \bar{\varepsilon}_1 + \bar{\varepsilon}_2 - W_{12} \bar{\varepsilon}_1 \bar{\varepsilon}_2 \right) \]
\[ Y_1 = \alpha_1^2 W_{12} \left( \bar{\varepsilon}_2 + 2 \bar{\varepsilon}_1 \right) - \bar{\varepsilon}_1 \bar{\varepsilon}_2 \]
\[ \alpha_1 = \sqrt{\varepsilon_1^2 + (W_{11} \Delta_1 + W_{12} \Delta_2)^2} \]

\[ \alpha_2 = \sqrt{\varepsilon_2^2 + (W_{12} \Delta_1 + W_{11} \Delta_2)^2 + 2W_{12}^2 \gamma^2} \]

Similarly

\[ F_{11} = -\frac{1}{2\pi} \left[ \left( \omega - \varepsilon_2 \right) \left( W_{11} \Delta_1 + W_{12} \Delta_2 \right) - \left( \omega - \varepsilon_1 \right) \left( W_{12} \Delta_1 + W_{11} \Delta_2 \right) \right] \]

On further simplification, one obtains

\[ F_{11} = \frac{1}{4\pi \alpha_1 (\alpha^2 - \alpha_2)} \left[ \frac{P + Q}{(\omega - \alpha)} + \frac{P - Q}{(\omega + \alpha)} \right] - \frac{1}{4\pi \alpha_2 (\alpha^2 - \alpha_2)} \left[ \frac{P + Q}{(\omega - \alpha_2)} + \frac{P - Q}{(\omega + \alpha_2)} \right] \]

Where

\[ P = -\alpha W_{12} \gamma \left( W_{11} \Delta_1 + W_{12} \Delta_2 \right) \left( W_{12} \Delta_1 + W_{11} \Delta_2 \right) \]

\[ Q = \alpha_2^2 \left( W_{11} \Delta_1 + W_{12} \Delta_2 \right) \left( W_{11} \Delta_1 + W_{12} \Delta_2 \right) \left( W_{12} \Delta_1 + W_{11} \Delta_2 \right) \left( W_{12} \Delta_1 + W_{11} \Delta_2 \right) \]

\[ P_1 = \alpha W_{12} \gamma \left( W_{11} \Delta_1 + W_{12} \Delta_2 \right) \left( W_{12} \Delta_1 + W_{11} \Delta_2 \right) \]

\[ Q_1 = -\alpha_2^2 \left( W_{11} \Delta_1 + W_{12} \Delta_2 \right) \left( W_{11} \Delta_1 + W_{12} \Delta_2 \right) \left( W_{12} \Delta_1 + W_{11} \Delta_2 \right) \left( W_{12} \Delta_1 + W_{11} \Delta_2 \right) \]

\[ \alpha_1 = \sqrt{\varepsilon_1^2 + (W_{11} \Delta_1 + W_{12} \Delta_2)^2} \]

\[ \alpha_2 = \sqrt{\varepsilon_2^2 + (W_{12} \Delta_1 + W_{11} \Delta_2)^2 + 2W_{12}^2 \gamma^2} \]

**Correlation functions**

Using the following relation\textsuperscript{19-23}

\[ \left\langle C_K^* C_K \right\rangle = \frac{1}{2\pi} \int_{-\infty}^{\infty} I_G(\omega) \exp\left[ -i \omega (t - t') \right] d\omega \]

Substituting \( t = t' \) we get

\[ \left\langle C_K^* C_K \right\rangle = \frac{1}{2\pi} \int_{-\infty}^{\infty} I_G(\omega) d\omega \]
Where

\[ I_{\omega} = \frac{i}{\varepsilon_{\omega} + 1} \left[ G_{1}\left(\omega + i \varepsilon\right) - G_{1}\left(\omega - i \varepsilon\right) \right] \]  

\[ \cdots (17) \]

and employing the following identity

\[ \lim_{\varepsilon \to 0} \left[ \frac{1}{\omega + i \varepsilon - E_{K}} - \frac{1}{\omega - i \varepsilon - E_{K}} \right] = 2\pi \delta(\omega - E_{K}) \]  

\[ \cdots (18) \]

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

\[ \langle C_{k}^{+} C_{k} \rangle = \left[ \frac{1}{4\pi} + \frac{1}{4\pi \alpha \alpha'_{k} \left( \alpha^2 - \alpha'^{2} \right)} \left( Y \tanh \left( \frac{\beta \alpha}{2} \right) + \alpha \alpha'_{k} Y W_{12} \gamma \tanh \left( \frac{\beta \alpha'}{2} \right) \right) \right] \]  

\[ \cdots (19) \]

where

\[ \frac{Y}{4\pi \alpha \alpha'_{k} \left( \alpha^2 - \alpha'^{2} \right)} = \frac{1}{4\pi} \left[ \epsilon_{k} - \frac{W_{12} \gamma}{\alpha \alpha'_{k}} \epsilon_{k} - \frac{\alpha W_{12} \gamma}{\left( \alpha^2 - \alpha'^{2} \right)} \right] \]  

\[ \cdots (20) \]

and

\[ \frac{Y W_{12} \gamma}{4\pi \alpha \alpha'_{k} \left( \alpha^2 - \alpha'^{2} \right)} = \frac{W_{12} \gamma}{4\pi \alpha \alpha'_{k} \left( \alpha^2 - \alpha'^{2} \right)} \left[ \epsilon_{k} + \epsilon_{k} \right] \]  

\[ \cdots (21) \]

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

\[ \langle C_{k}^{+} C_{k} \rangle = \left[ \frac{1}{4\pi \left( \alpha^2 - \alpha'^{2} \right)} \left( \frac{W \alpha^2 - \left( W \epsilon^2 + W_{12} \gamma (W \epsilon + W') \right) \tanh \left( \frac{\beta \alpha}{2} \right)}{\alpha} \right) \right. \]  

\[ \left. - \frac{W \alpha'^{2} - \left( W \epsilon^2 + W_{12} \gamma (W \epsilon + W') \right) \tanh \left( \frac{\beta \alpha'}{2} \right)}{\alpha'} \right] \]  

\[ \cdots (22) \]

Where

\[ W' = W_{12} \Delta_{1} + W_{11} \Delta_{2} \]  

\[ \cdots (23) \]

\[ W = W_{11} \Delta_{1} + W_{12} \Delta_{2} \]  

\[ \cdots (24) \]

**Physical properties**

**Superconducting order parameter**

Superconducting order parameter (\( \Delta \)) is given by –
\[ \Delta = \sum_k |C_k C_k| \]  

...\(25\)

Now using Eq. (22) we obtain

\[ \Delta = k \sum_k \frac{1}{4\pi(\alpha_1^2 - \alpha_2^2)} \left[ \frac{W\alpha_1^2 - W\varepsilon_2^2 + W\varepsilon_2 + W\frac{\varepsilon_2}{\mu}}{\alpha_1} \tanh\left( \frac{\beta\alpha_1}{2} \right) - \frac{W\alpha_2^2 - W\varepsilon_2^2 + W\varepsilon_2 + W\frac{\varepsilon_2}{\mu}}{\alpha_2} \tanh\left( \frac{\beta\alpha_2}{2} \right) \right] \]

...\(26\)

Applying identity,

\[ \sum_k = 2N(0) \int_0^\infty d\varepsilon \]  

...\(27\)

We get

\[ \Delta = 2N(0) k \int_0^\infty \left[ \frac{W\alpha_1^2 - W\varepsilon_2^2 + W\varepsilon_2 + W\frac{\varepsilon_2}{\mu}}{4\pi(\alpha_1^2 - \alpha_2^2)} \left( \frac{1}{\alpha_1} \tanh\left( \frac{\beta\alpha_1}{2} \right) - \frac{1}{\alpha_2} \tanh\left( \frac{\beta\alpha_2}{2} \right) \right) \right] d\varepsilon \]  

...\(28\)

Where \(W, W', \alpha_1\) and \(\alpha_2\) are defined in previous section and

\[ \alpha_1^2 - \alpha_2^2 = \varepsilon_2^2 - \varepsilon_2^2 + (W_1D_1 + W_1D_2)^2 - (W_1D_1 + W_1D_2)^2 - 2W_1^2 \]

\[ \varepsilon_1 = \varepsilon_1 - \frac{W_1}{2} \]

\[ \varepsilon_2 = \varepsilon_2 - \frac{W_1}{2} \]

**Case 1:**

For \(\Delta_1\), applying \(\varepsilon_2 = \varepsilon_2\) and \(\Delta_2 = 0\) in Eq. (28), we get,
\[ \Delta_1 = 2N(0) \int_0^\infty \left[ \frac{W_i \Delta_i}{4 \pi (a_1^2 - a_2^2)} \left\{ a_1 \tanh \left( \frac{\beta a_1}{2} \right) - a_2 \tanh \left( \frac{\beta a_2}{2} \right) \right\} \right] d e_i \] ... (29)

\[ \frac{1}{|g|N(0)} = \frac{h_{\alpha_0}}{2 \pi \Delta_2} \int_0^\infty \left( \frac{e_2 - W_{11}}{2} \right)^2 + W_{11} \left( e_2 - W_{11} \right) - W_{11} \Delta_2^2 \right) \tanh \frac{h_{\alpha_0} W_{11} \Delta_2^2}{2} d e_2 \] ...

Case 2:

For \( \Delta_2 \), applying \( e_1 = 0 \) and \( \Delta_1 = 0 \) in Eq. (28), we get

\[ \Delta_2 = 2N(0) \int_0^\infty \left[ \frac{W_i \Delta_i}{4 \pi (a_1^2 - a_2^2)} \left\{ a_1 \tanh \left( \frac{\beta a_1}{2} \right) - a_2 \tanh \left( \frac{\beta a_2}{2} \right) \right\} \right] d e_2 \] ... (31)

\[ \frac{1}{|g|N(0)} = \frac{h_{\alpha_0}}{2 \pi \Delta_2} \int_0^\infty \left( \frac{e_2 - W_{11}}{2} \right)^2 + W_{11} \left( e_2 - W_{11} \right) - W_{11} \Delta_2^2 \right) \tanh \frac{h_{\alpha_0} W_{11} \Delta_2^2}{2} d e_2 \] ...

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

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Superconducting transition temperature</td>
<td>39 K</td>
<td>1</td>
</tr>
<tr>
<td>Phonon energy ($\epsilon_1$)</td>
<td>0.06 eV</td>
<td>25</td>
</tr>
<tr>
<td>Phonon energy ($\epsilon_2$)</td>
<td>0.05 eV</td>
<td>25</td>
</tr>
<tr>
<td>Density of states at the Fermi surface</td>
<td>3.093 / eV.atom</td>
<td>25</td>
</tr>
<tr>
<td>Pairing interaction $W_{11} = W_{22}$ intra-band</td>
<td>0.3 eV.cell</td>
<td>13</td>
</tr>
<tr>
<td>Pairing interaction $W_{12} = W_{21}$ inter-band</td>
<td>0.0001 eV.cell</td>
<td>13</td>
</tr>
<tr>
<td>No. of atoms per unit volume</td>
<td>$5 \times 10^{28}$/ m$^3$</td>
<td>31</td>
</tr>
<tr>
<td>Cell parameter</td>
<td>$a = 3.086$ Å, $b = 3.524$ Å</td>
<td>26</td>
</tr>
<tr>
<td>Boltzmann constant</td>
<td>$1.38 \times 10^{-23}$ J/K</td>
<td>-</td>
</tr>
<tr>
<td>Mass of electron</td>
<td>$9.1 \times 10^{-31}$ Kg</td>
<td>-</td>
</tr>
</tbody>
</table>

**Electronic specific heat**

The electronic specific heat per atom of a superconductor is given by $^{3,19-24}$ –

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

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

$$\sum_K = N(0) \int d \epsilon_K \quad \ldots(34)$$

One obtain

$$C_{es} = \frac{2N(0)}{N} \int_0^{\beta \hbar} \frac{d \epsilon_K}{8\pi k_B T^3 (\alpha_1^2 - \alpha_2^2)} \left[ \langle \alpha_1^2 - \alpha_2^2 \rangle \tilde{\epsilon}_1 - W_{12} \gamma (\alpha_1^2 + \tilde{\epsilon}_1 \tilde{\epsilon}_2) \sec \frac{\beta \alpha_1}{2} \right] \quad \ldots(35)$$
Case 1:
For $C_{\alpha},$ applying $\varepsilon_2 = 0$ and $\Delta_2 = 0$ in Eq. (35) we get,

\[
\begin{align*}
C_{\alpha} &= \frac{N(0)}{N} \frac{1}{4 \hbar^2} \\
&= \frac{N(0)}{N} \frac{1}{4 \hbar^2} \left[ \int_0^{\lambda_{\phi_0}} \varepsilon_{\alpha} \left( e_{\alpha} - \frac{W_{11}}{2} \right) \text{sech}^2 \frac{\hbar^2}{2 \lambda_{\phi_0}} \left( e_{\alpha} - \frac{W_{11}}{2} \right)^2 + \varepsilon_{\alpha} \left( \left( e_{\alpha} - \frac{W_{11}}{2} \right)^2 + \Delta_1^2 \right) \right] \end{align*}
\]

... (36)

Case 2:
For $C_{\alpha},$ applying $\varepsilon_1 = 0$ and $\Delta_1 = 0$ in Eq. (35), we get

\[
\begin{align*}
C_{\alpha} &= \frac{N(0)}{N} \frac{1}{4 \hbar^2} \\
&= \frac{N(0)}{N} \frac{1}{4 \hbar^2} \left[ \int_0^{\lambda_{\phi_0}} \varepsilon_{\alpha} \left( e_{\alpha} - \frac{W_{11}}{2} \right) \text{sech}^2 \frac{\hbar^2}{2 \lambda_{\phi_0}} \left( e_{\alpha} - \frac{W_{11}}{2} \right)^2 + \varepsilon_{\alpha} \left( \left( e_{\alpha} - \frac{W_{11}}{2} \right)^2 + \Delta_2^2 \right) \right] \end{align*}
\]

... (37)

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

Numerical calculations

We now evaluate numerically $\Delta$ and $C_{\alpha}$ using the parameters given in Table 1 for MgB$_2$.

Superconducting order parameter ($\Delta$)

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

\[ W_{11} = W_{22} = 0.3 \text{ eV. cell} = 9.6 \times 10^{-21} \text{J} \]
\[ W_{12} = W_{21} = z \text{ eV.cell} = z \times 32 \times 10^{-21} \text{J} \]
\[ \gamma = (-) 0.01753 \]
\[ \epsilon_1 = 0.06 \text{ y eV} = 9.6 \times 10^{-21} \text{y J} \]
\[ k_B = 1.38 \times 10^{-23} \text{J/K} \]
\[ \hbar \omega_D = 0.06 \text{eV} \]
\[ \Delta_1 = x \]

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

\[
\frac{1}{|g|} \ln(0) = 1.528 \times 10^{-21} \int_{y=0}^{y=1} \frac{\sqrt{(y-0.5)^2 + x^2}}{\sqrt{(y-0.5)^2 + (1 - 11.11z^2)x^2 - 0.0068z^2}} \tanh \left( \frac{347.82}{\gamma(y-0.5)^2 + x^2} \right) dy 
+ 0.2978 \times 10^{-21} z^2 \int_{y=0}^{y=1} \frac{\sqrt{(y-0.5)^2 + x^2}}{\sqrt{(y-0.5)^2 + (1 - 11.11z^2)x^2 - 0.0068z^2}} \tanh \left( \frac{347.82}{\gamma(y-0.5)^2 + x^2} \right) dy 
- 5.096 \times 10^{-21} z^2 \int_{y=0}^{y=1} \frac{\sqrt{x^2 + 0.000614}}{\sqrt{(1 - 11.11z^2)x^2 - 0.0068z^2}} \tanh \left( \frac{11.954}{\gamma(y-0.5)^2 + x^2} \right) dy 
+ 0.000614 \int_{y=0}^{y=1} \frac{\sqrt{x^2 + 0.000614}}{\sqrt{(1 - 11.11z^2)x^2 - 0.0068z^2}} \tanh \left( \frac{11.954}{\gamma(y-0.5)^2 + x^2} \right) dy
\]

\[ \cdots(38) \]

**Superconducting order parameter 2 (\Delta_2)**

Choosing
\[ W_{11} = W_{22} = 0.3 \text{ eV.cell} = 9.6 \times 10^{-21} \text{J} \]
\[ W_{12} = W_{21} = z \text{ eV.cell} = z \times 32 \times 10^{-21} \text{J} \]
\[ \gamma = (-) 0.01753 \]
\[ \epsilon_2 = 0.05 \text{ y eV} = 8 \times 10^{-21} \text{y J} \]
\[ k_B = 1.38 \times 10^{-23} \text{J/K} \]
\[ \hbar \omega_D = 0.05 \text{ eV} \]
\[ \Delta_2 = x \]

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

\[
\frac{1}{|g|} \ln(0) = 1.273 \times 10^{-21} / x \tanh \left( \frac{115.4}{\gamma} \right) z^2 + \frac{10.24 + x^2[22.16 - 1024z^2]}{23.04 + x^2[22.16 - 1024z^2]} + 0.629z^2 
- x^2 \left( \frac{3}{\gamma} \frac{[1 - 11.11z^2]}{[1 - 11.11z^2]^2 + 0.0068z^2} \right) \tanh \left( \frac{289.85}{\gamma(y-0.6)^2 + 1.44x^2 + 0.00983z^2} \right) dy 
+ 0.3573 \times 10^{-21} z^2 \int_{y=0}^{y=1} \frac{(y-0.6)}{\sqrt{(y-0.6)^2 + 1.44x^2 + 0.00983z^2}} \tanh \left( \frac{289.85}{\gamma(y-0.6)^2 + 1.44x^2 + 0.00983z^2} \right) dy 
+ 0.7643 \times 10^{-21} z^2 \int_{y=0}^{y=1} \frac{1}{\sqrt{(y-0.6)^2 + 1.44x^2 + 0.00983z^2}} \tanh \left( \frac{289.85}{\gamma(y-0.6)^2 + 1.44x^2 + 0.00983z^2} \right) dy
\]

\[ \cdots(39) \]
Solving numerically Eq. (38) and (39), we obtain variations of superconducting order parameters ($\Delta_1$, $\Delta_2$ and $\Delta$) 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 ($\Delta_1$) for magnesium diboride (MgB$_2$) system**

<table>
<thead>
<tr>
<th>Temp. (K)</th>
<th>$\Delta_1$ (Theoretical) (meV)</th>
<th>$\Delta_1$ (Experimental) (meV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>0.6241</td>
<td>2.90</td>
</tr>
<tr>
<td>10</td>
<td>0.6236</td>
<td>2.86</td>
</tr>
<tr>
<td>15</td>
<td>0.6164</td>
<td>2.82</td>
</tr>
<tr>
<td>20</td>
<td>0.5941</td>
<td>2.70</td>
</tr>
<tr>
<td>25</td>
<td>0.5487</td>
<td>2.20</td>
</tr>
<tr>
<td>30</td>
<td>0.4702</td>
<td>1.70</td>
</tr>
<tr>
<td>32</td>
<td>0.4251</td>
<td>1.35</td>
</tr>
<tr>
<td>35</td>
<td>0.3331</td>
<td>0.88</td>
</tr>
<tr>
<td>36</td>
<td>0.2922</td>
<td>0.72</td>
</tr>
<tr>
<td>37</td>
<td>0.2414</td>
<td>0.45</td>
</tr>
<tr>
<td>38</td>
<td>0.1725</td>
<td>0.20</td>
</tr>
<tr>
<td>39</td>
<td>0.0056</td>
<td>0.00</td>
</tr>
</tbody>
</table>

**Table 3: Superconducting order parameter ($\Delta_2$) for magnesium diboride (MgB$_2$) system**

<table>
<thead>
<tr>
<th>Temp. (K)</th>
<th>$\Delta_2$ (Theoretical) (meV)</th>
<th>$\Delta_2$ (Experimental) (meV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>6.1169</td>
<td>7.20</td>
</tr>
<tr>
<td>10</td>
<td>5.7075</td>
<td>7.16</td>
</tr>
<tr>
<td>15</td>
<td>4.5750</td>
<td>6.93</td>
</tr>
<tr>
<td>20</td>
<td>2.8313</td>
<td>6.40</td>
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<tr>
<td>25</td>
<td>1.8225</td>
<td>5.70</td>
</tr>
<tr>
<td>30</td>
<td>1.0531</td>
<td>4.15</td>
</tr>
<tr>
<td>32</td>
<td>0.7638</td>
<td>3.43</td>
</tr>
<tr>
<td>35</td>
<td>0.3116</td>
<td>2.30</td>
</tr>
<tr>
<td>36</td>
<td>0.1971</td>
<td>1.90</td>
</tr>
<tr>
<td>37</td>
<td>0.1142</td>
<td>1.20</td>
</tr>
<tr>
<td>38</td>
<td>0.0513</td>
<td>0.60</td>
</tr>
<tr>
<td>39</td>
<td>0.0006</td>
<td>0.00</td>
</tr>
</tbody>
</table>
Table 4: Superconducting order parameter ($\Delta = \Delta_1 + \Delta_2$) for magnesium diboride (MgB$_2$) system

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

Fig. 1: Variations of superconducting order parameter ($\Delta_1$) with temperature for magnesium diboride (MgB$_2$) system
Fig. 2: Variations of superconducting order parameter ($\Delta_2$) 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 $C_{es}$

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

$W_{12} = W_{21} = z \text{ eV. cell} = z \times 32 \times 10^{-21} \text{J}$

$\gamma = (-) 0.01753$

$\epsilon_1 = 0.06 y \text{ eV} = 9.6 \times 10^{-21} y \text{ J}$

$k_B = 1.38 \times 10^{-23} \text{ J/K}$
\[ \hbar \omega_D = 0.06 \text{ eV} \quad \Delta_1 = x \]
\[ \text{N}(0) = 3.093 / \text{eV.atom} \quad \text{N} = 5 \times 10^{28}/\text{m}^3 \]

We obtain

\[
C_n^1 = \frac{32.8 \times 10^{-16}}{T^2} \left[ 1.54 \int_{x=0}^{x=1} \left[ (y-0.5) \text{sec} h^2 \frac{347.82}{T} \frac{\sqrt{y-0.5} + x}{y} \right] \frac{y dy}{y-0.5} + \frac{\sqrt{y-0.5} + x}{y} \right] \]
\[
+ 0.09x^2 \int_{0}^{x} \left[ (y-0.5)^2 + x^2 \text{sec} h^2 \frac{347.82}{T} \frac{\sqrt{y-0.5} + x}{y} \right] \frac{y dy}{y-0.5} + \frac{\sqrt{y-0.5} + x}{y} \right] - z \left[ (y + 0.00614) \text{sec} h^2 \frac{1159.4}{T} (y + 0.00614) \sqrt{y-0.5} + \frac{\sqrt{y-0.5} + x}{y} \right] \frac{y dy}{y-0.5} + \frac{\sqrt{y-0.5} + x}{y} \right] \space (40) \]

Substituting following values in Eq. (37) for \( C_n^2 \)

\[ W_{11} = W_{22} = 0.3 \text{ eV.cell} = 9.6 \times 10^{-21} \text{J} \]
\[ W_{12} = W_{21} = z \text{ eV.cell} = z \times 32 \times 10^{-21} \text{J} \quad \gamma = (-) 0.01753 \]
\[ \epsilon_2 = 0.05 \text{ y eV} = 8 \times 10^{-21} \text{ y J} \quad k_B = 1.38 \times 10^{-23} \text{ J/K} \]
\[ \hbar \omega_D = 0.05 \text{eV} \quad \Delta_2 = x \]
\[ \text{N}(0) = 3.093 / \text{eV.atom} \quad \text{N} = 5 \times 10^{28}/\text{m}^3 \]

We obtain

\[
C_n^2 = \frac{2.05 \times 10^{-16}}{T^2} \left[ -16e^2 \text{ sec} h^2 \frac{1159.4}{T} \left( \int_{0}^{y} \frac{y^2}{y-0.5} \right) + 1.44x^2 - 11.11x^2 \text{sec} h^2 \frac{x^2}{y-0.5} \right] \int_{0}^{y} \frac{y}{y-0.5} \text{sec} h^2 \frac{289.85}{T} \left( y - 0.5 \right)^2 + 1.44x^2 - 0.00683x^2 \text{sec} h^2 \frac{1159.4}{T} \text{sec} h^2 \frac{x^2}{y-0.5} \right] \frac{y dy}{y-0.5} + \frac{\sqrt{y-0.5} + x}{y} \right] \space (41) \]
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 ($C_{es}$) for magnesium diboride (MgB$_2$) system**

<table>
<thead>
<tr>
<th>Temp. (K)</th>
<th>$C_{es}$ (Theoretical) = $C_1^{es} + C_2^{es}$</th>
<th>$C_{es}$ (Experimental)</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>0.00006</td>
<td>1.9</td>
</tr>
<tr>
<td>10</td>
<td>0.2792</td>
<td>10.1</td>
</tr>
<tr>
<td>15</td>
<td>3.6511</td>
<td>29.1</td>
</tr>
<tr>
<td>20</td>
<td>12.8391</td>
<td>45.3</td>
</tr>
<tr>
<td>25</td>
<td>27.9675</td>
<td>64.0</td>
</tr>
<tr>
<td>30</td>
<td>48.4162</td>
<td>91.8</td>
</tr>
<tr>
<td>32</td>
<td>57.9393</td>
<td>99.2</td>
</tr>
<tr>
<td>35</td>
<td>73.5297</td>
<td>113.9</td>
</tr>
<tr>
<td>36</td>
<td>79.0362</td>
<td>112.1</td>
</tr>
<tr>
<td>37</td>
<td>84.7204</td>
<td>110.7</td>
</tr>
<tr>
<td>38</td>
<td>90.5759</td>
<td>105.3</td>
</tr>
<tr>
<td>39</td>
<td>96.5675</td>
<td>101.2</td>
</tr>
</tbody>
</table>

**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 $\Delta_1$, $\Delta_2$ 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 $\Delta_1$, $\Delta_2$ 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$^{29-36}$

REFERENCES


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