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Theoretical Study of Specific Heat and Density of States of MgB_2 Superconductor in Two Band Models

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ABSTRACT

MgB_2 with $T_c \approx 40$ K, is a record-breaking compound among the s-p metals and alloys. It appears that this material is a rare example of the two band electronic structures, which are weakly connected with each other. Experimental results clearly reveal that boron sub-lattice conduction band is mainly responsible for superconductivity in this simple compound. Experiments such as tunneling spectroscopy, specific heat measurements, and high resolution spectroscopy show that there are two superconducting gaps. Considering a canonical two band BCS Hamiltonian containing a Fermi Surface of π- and σ-bands and following Green's function technique and equation of motion method, we have shown that MgB_2 possess two superconducting gaps. It is also pointed out that the system admits a precursor phase of Cooper pair droplets that undergoes a phase locking transition at a critical temperature below the mean field solution. Study of specific heat and density of states is also presented. The agreement between theory and experimental results for specific heat is quite convincing. The paper is organized in five sections: Introduction, Model Hamiltonian, Physical properties, Numerical calculations, Discussion and conclusions.

Keywords: Green's Function; *p* and *d* Holes; Specific Heat; Density of States

1. Introduction

The surprising discovery of superconductivity in the novel system MgB_2 with $T_c = 39$ K by Nagamatsu *et al*. [1] has stimulated new excitement in condensed matter physics. This discovery certainly revived the interest in the field of superconductivity especially in non-oxides, and initiated a search for superconductivity in related boron compounds [2]. Its high critical temperature gives hope for obtaining even higher T_c for similar compounds.

The crystal structure of MgB_2 is very simple. It is composed of layers of boron and magnesium, alternating along the c-axis. Each boron layer has a hexagonal lattice similar to that of graphite. The magnesium atoms are arranged between the boron layers in the centers of the hexagons. This has allowed to perform consistent calculations of its electronic structure. Band structure calculations of MgB_2 show that there are at least two types of nearly separated bands with two superconducting gaps in the excitation spectrum at the Fermi surface. The first one is a heavy hole band, built up of boron σ orbitals. The second one is the broader band with a smaller effective mass, built up mainly of π boron orbitals [3-7].

It is now well established that MgB_2 is an anisotropic two-gap superconductor [4]. The gap ratio $2\Delta/k_BT_c$ for the larger gap $\overline{\Delta}_d$ is 7.6. For the smaller gap $\overline{\Delta}_p$, this ratio is around 2.78, so that $\overline{\Delta}_d/\overline{\Delta}_p \approx 2.7$. Seemingly, both the energy gaps have s-wave symmetries, the larger gap is highly anisotropic, while the smaller one is either isotropic or slightly anisotropic. The induced character of $\overline{\Delta}_p$ manifests itself in its temperature dependence. The larger energy gap $\overline{\Delta}_d$ occurs in σ-orbital band, while $\overline{\Delta}_p$ in the π-orbital band. For a simplified description, single effective σ- and π-bands can be introduced.

The Fermi surface consists of four sheets: two three dimensional sheets form the π bonding and antibonding bands $(2p_z)$, and two nearly cylindrical sheets form the two-dimensional σ-band $(2p_{x,y})$ [4,8]. There is a large difference in the electron-phonon coupling on different Fermi surface sheets and this leads to multiband description of superconductivity. The average electronphonon coupling strength is found to have small values [9-11]. Ummarino *et al*. [12] proposed that MgB_2 is a weak coupling two band phononic system where the Coulomb pseudopotential and the interchannel paring mechanism are key terms to interpret the superconducting state. Garland [13] has remarked that Coulomb potential in the *d*-orbitals of the transition metal reduce the isotope exponent, whereas sp-metals generally shows a nearly full isotope effect. Clearly, like sp metal, for MgB_2 the Coulomb effect cannot be considered to explain the reduction

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of isotope exponent.

It is quite natural to describe a two-gap superconductor by means of a two-band model with interband coupling [14,15]. For MgB_2, an approach of such kind is also directly proposed by the nature of the electron spectrum mentioned. There is a number of two band type approaches for superconductivity in MgB_2 [16]. We may note that two band models have been exploited in various realizations for high-T_c cuprate superconductivity [16,17].

Liu *et al*. [4] pointed the role of the electron-phonon interaction between effective σ- and π-bands in the two gap system MgB_2. In the present study, we use σ-π interband coupling with a strong σ-interband contribution of electron-phonon and Coulobmic nature. Following Liu *et al*. [4], the interband interaction is considered to be repulsive (an advantage of two band models) corresponding to electron-electron interaction.

Using two band models, we study the basic MgB_2 superconductivity characteristics, specific heat and density of states and compare the theoretical results qualitatively with the available experimental data.

2. The Model Hamiltonian

The model Hamiltonian has the form [18]

$$H = H_0^p + H_0^d + H_{pd} \tag{1}$$

where

$$\begin{aligned} H_0^p &= \sum_p \in_p \left(C_{p\uparrow}^+ C_{p\uparrow} + C_{-p\downarrow}^+ C_{-p\downarrow} \right) \\ &\quad + \Delta_{pp}^+ \sum_p C_{-p\downarrow} C_{p\uparrow} + \Delta_{pp} \sum_p C_{p\uparrow}^+ C_{-p\downarrow}^+ \end{aligned} \tag{2}$$

$$\begin{aligned} H_0^d &= \sum_d \in_d \left(C_{d\uparrow}^+ C_{d\uparrow} + C_{-d\downarrow}^+ C_{-d\downarrow} \right) \\ &\quad + \Delta_{dd}^+ \sum_d C_{-d\downarrow} C_{d\uparrow} + \Delta_{dd} \sum_d C_{d\uparrow}^+ C_{-d\downarrow}^+ \end{aligned} \tag{3}$$

and

$$\begin{aligned} H_{pd} &= V_{pd} \left\langle C_{p\uparrow}^+ C_{-p\downarrow}^+ \right\rangle \sum_d C_{-d\downarrow} C_{d\uparrow} \\ &\quad + V_{pd} \left\langle C_{-d\downarrow} C_{d\uparrow} \right\rangle \sum_p C_{p\uparrow}^+ C_{-p\downarrow}^+ \\ &\quad + V_{pd} \left\langle C_{d\uparrow}^+ C_{-d\downarrow}^+ \right\rangle \sum_p C_{-p\downarrow} C_{p\uparrow} \\ &\quad + V_{pd} \left\langle C_{-p\downarrow} C_{p\uparrow} \right\rangle \sum_d C_{d\uparrow}^+ C_{-d\downarrow}^+ \end{aligned} \tag{4}$$

Here p and d are momentum labels in the π- and σ-bands respectively with energies $\in_p$ and $\in_d$, μ is the common chemical potential. Each band has its proper pairing interaction V_{pp} and V_{dd}, while the pair interchange between the two bands is assured by V_{pd} term.

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

$$\in_p = \in_p^0 - \mu, \in_d = \in_d^0 - \mu$$

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

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

Further we define

$$\begin{aligned} \Delta_1^+ &= V_{pd} \left\langle C_{p\uparrow}^+ C_{-p\downarrow}^+ \right\rangle \\ \Delta_2^+ &= V_{pd} \left\langle C_{d\uparrow}^+ C_{-d\downarrow}^+ \right\rangle \end{aligned} \tag{5}$$

Now H_{pd} in Equation (1) read as

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

Final Hamiltonian can be written as

$$\begin{aligned} H &= \sum_p \in_p \left(C_{p\uparrow}^+ C_{p\uparrow} + C_{-p\downarrow}^+ C_{-p\downarrow} \right) + \Delta_{pp}^+ \sum_p C_{-p\downarrow} C_{p\uparrow} \\ &\quad + \Delta_{pp} \sum_p C_{p\uparrow}^+ C_{-p\downarrow}^+ + \sum_d \in_d \left(C_{d\uparrow}^+ C_{d\uparrow} + C_{-d\downarrow}^+ C_{-d\downarrow} \right) \\ &\quad + \Delta_{dd}^+ \sum_d C_{-d\downarrow} C_{d\uparrow} + \Delta_{dd} \sum_d C_{d\uparrow}^+ C_{-d\downarrow}^+ \\ &\quad + \Delta_1^+ \sum_d C_{-d\downarrow} C_{d\uparrow} + \Delta_2 \sum_p C_{-p\downarrow}^+ C_{p\uparrow}^+ \\ &\quad + \Delta_2^+ \sum_p C_{-p\downarrow} C_{p\uparrow} + \Delta_1 \sum_d C_{d\uparrow}^+ C_{-d\downarrow}^+ \end{aligned} \tag{6}$$

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

2.1. Green's Functions

In order to study the physical properties, we define the following normal and anomalous Green's functions [18-28]:

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

Following equation of motion method, we obtain Green's functions as follows. In obtaining Green's functions, we have assumed

$$\left(\Delta_{pp} + \Delta_2 \right) = \overline{\Delta}_p \quad \text{and} \quad \Delta_{pp}^+ \cong \Delta_{pp}$$

$$\left(\Delta_{dd} + \Delta_1 \right) = \overline{\Delta}_d \quad \text{and} \quad \Delta_{dd}^+ \cong \Delta_{dd}$$

Then

$$\left(\Delta_{pp}^{+}+\Delta_{2}^{+}\right)\cong\left(\Delta_{pp}+\Delta_{2}\right)=\overline{\Delta}_{p}$$
$$\left(\Delta_{dd}^{+}+\Delta_{1}^{+}\right)\cong\left(\Delta_{dd}+\Delta_{1}\right)=\overline{\Delta}_{d} \quad (8)$$

1) Green's functions for π-band

$$\left\langle\left\langle C_{p\uparrow},C_{p\uparrow}^{+}\right\rangle\right\rangle=\frac{\left(\omega+\in_{p}\right)}{\left(\omega^{2}-E_{p}^{2}\right)} \quad (9)$$

$$\left\langle\left\langle C_{p\uparrow}^{+},C_{-p\downarrow}^{+}\right\rangle\right\rangle=-\frac{\overline{\Delta}_{p}}{\left(\omega^{2}-E_{p}^{2}\right)} \quad (10)$$

2) Green's functions for σ-band

$$\left\langle\left\langle C_{d\uparrow},C_{d\uparrow}^{+}\right\rangle\right\rangle=\frac{\left(\omega+\in_{d}\right)}{\left(\omega^{2}-E_{d}^{2}\right)} \quad (11)$$

$$\left\langle\left\langle C_{d\uparrow}^{+},C_{-d\downarrow}^{+}\right\rangle\right\rangle=-\frac{\overline{\Delta}_{d}}{\left(\omega^{2}-E_{d}^{2}\right)} \quad (12)$$

2.2. The Correlation Functions

Using the following relation [23-27],

$$\left\langle B(t')A(t)\right\rangle = \underset{\in\to 0}{\text{Limit}}\frac{i}{2\pi}\int_{-\infty}^{+\infty}\frac{\left\langle\left\langle A(t');B(t')\right\rangle\right\rangle_{\omega+i\in}-\left\langle\left\langle A(t');B(t')\right\rangle\right\rangle_{\omega-i\in}}{\mathrm{e}^{\beta\omega}+1}\times\exp\left(-i\omega\left(t-t'\right)\right)\mathrm{d}\omega \quad (13)$$

and employing the following identity,

$$\underset{\in\to 0}{\text{Limit}}\left(\frac{1}{\omega+i\in-E_{K}}-\frac{1}{\omega-i\in-E_{K}}\right)=2\pi i\delta\left(\omega-E_{K}\right)$$

we obtain the correlation functions for the Green's functions given by Equations (9) and (10) as:

$$\left\langle C_{p\uparrow}^{+}C_{p\uparrow}\right\rangle=f\left(\alpha_{2}\right)+\left[\frac{\alpha_{1}-\in_{P}}{\left(\alpha_{1}-\alpha_{2}\right)}\right]\left[f\left(\alpha_{1}\right)-f\left(\alpha_{2}\right)\right] \quad (14)$$

$$\left\langle C_{p\uparrow}^{+}C_{-p\downarrow}^{+}\right\rangle=\frac{\overline{\Delta}_{p}}{\left(\alpha_{1}-\alpha_{2}\right)}\left[f\left(\alpha_{1}\right)-f\left(\alpha_{2}\right)\right] \quad (15)$$

where

$$\begin{aligned}\alpha_{1}&=+\sqrt{\in_{p}^{2}+\Delta_{pp}^{2}+\Delta_{2}^{2}+\Delta_{pp}^{+}\Delta_{2}+\Delta_{2}^{+}\Delta_{pp}}\\&=+\sqrt{\in_{p}^{2}+\left(\Delta_{pp}+\Delta_{2}\right)^{2}}=+\sqrt{\in_{p}^{2}+\overline{\Delta}_{p}^{2}}\\\alpha_{2}&=-\sqrt{\in_{p}^{2}+\Delta_{pp}^{2}+\Delta_{2}^{2}+\Delta_{pp}^{+}\Delta_{2}+\Delta_{2}^{+}\Delta_{pp}}\\&=-\sqrt{\in_{p}^{2}+\left(\Delta_{pp}+\Delta_{2}\right)^{2}}-\sqrt{\in_{p}^{2}+\overline{\Delta}_{p}^{2}}\end{aligned} \quad (16)$$

and $f\left(\alpha_{1}\right)\&\,f\left(\alpha_{2}\right)$ are Fermi functions.

Similarly correlation functions for Green's functions (11) and (12) for σ holes are obtained.

One can define the two superconducting order parameters related to the correlation functions corresponding to Green's functions $\left\langle\left\langle C_{p\uparrow}^{+},C_{-p\downarrow}^{+}\right\rangle\right\rangle$ and $\left\langle\left\langle C_{d\uparrow}^{+},C_{-d\downarrow}^{+}\right\rangle\right\rangle$ for π- and σ-bands respectively. In a similar manner electronic specific heat can also be defined related to both π- and σ-bands.

3. Physical Properties

3.1. Superconducting Order Parameters

Gap parameter $\overline{\Delta}$ is the superconducting order parameter, which can be determined self consistently from the gap equations

$$\overline{\Delta}_{p}=\Delta_{pp}+\Delta_{2}\equiv V_{pp}f_{p}+V_{pd}f_{d} \quad (17)$$

$$\overline{\Delta}_{d}=\Delta_{dd}+\Delta_{1}\equiv V_{pd}f_{p}+V_{dd}f_{d} \quad (18)$$

In a matrix form, the order parameter for the superconducting state is given by [19]

$$\overline{\Delta}_{i}=\sum_{j}V_{ij}G\left(\overline{\Delta}_{j}\right)\overline{\Delta}_{j} \quad (19)$$

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

$$G\left(\overline{\Delta}_{p}\right)=N_{p}\left(0\right)\int_{0}^{\hbar\omega_{p}}\frac{\mathrm{d}\in_{p}}{E_{p}}\tanh\frac{E_{p}}{2k_{B}T} \quad (20)$$

$$G\left(\overline{\Delta}_{d}\right)=N_{d}\left(0\right)\int_{0}^{\hbar\omega_{d}}\frac{\mathrm{d}\in_{d}}{E_{d}}\tanh\frac{E_{d}}{2k_{B}T} \quad (21)$$

Here $N_{p}\left(0\right)$ and $N_{d}\left(0\right)$ are density of states for π- and σ-bands respectively at the Fermi level.

There are two superconducting gaps corresponding to π- and σ-bands in this interband model. One can write the equations for superconducting gaps corresponding to π- and σ-bands as follows

$$\overline{\Delta}_{p}=V_{pd}G\left(\overline{\Delta}_{d}\right)\overline{\Delta}_{d}+V_{pp}G\left(\overline{\Delta}_{p}\right)\overline{\Delta}_{p} \quad (22)$$

$$\overline{\Delta}_{d}=V_{dp}G\left(\overline{\Delta}_{p}\right)\overline{\Delta}_{p}+V_{dd}G\left(\overline{\Delta}_{d}\right)\overline{\Delta}_{d} \quad (23)$$

where V_{pp} and V_{dd} is pairing interaction for π- and σ-bands respectively, while the pair interchange between the two bands is assured by the V_{pd} term. The quantity V_{pd} has been supposed to be operative and constant in the energy interval for higher band and lower band, keeping in mind the integration ranges, the gap parameter satisfy the system if the interband interactions are missing, *i.e.* $V_{pp}=V_{dd}=0$, the transition is solely induced by the interband interaction [16] and given by

$$k_B T_c = 1.14\hbar\omega_c \exp\left[-\frac{1}{\left|V_{pd}\sqrt{N_p N_d}\right|}\right] \tag{24}$$

Using Equations (24), we can write the simultaneous equation as

$$\frac{V_{pd}G\left(\bar{\Delta}_d\right)}{\left[1-V_{pp}G\left(\bar{\Delta}_p\right)\right]}\times\frac{V_{pd}G\left(\bar{\Delta}_p\right)}{\left[1-V_{pp}G\left(\bar{\Delta}_d\right)\right]}=1 \tag{25}$$

$$\bar{\Delta}=\bar{\Delta}_p+\bar{\Delta}_d=\left(V_{pd}+V_{pp}\right)\left(G\left(\bar{\Delta}_p\right)\bar{\Delta}_p+G\left(\bar{\Delta}_d\right)\bar{\Delta}_d\right) \tag{26}$$

3.2. Electronic Specific Heat (C_{es})

The electronic specific heat per atom of a superconductor is determined from the following relation [3,23-28],

1) For π-band

$$C_{es}^{p}=\frac{\partial}{\partial T}\frac{1}{N}\sum_{p}2\left(\in_p-\mu\right)\left\langle C_{p\uparrow}^{+}C_{p\uparrow}\right\rangle \tag{27}$$

where $\in_p$ is the energy of π-band and μ is the common chemical potential.

Substituting $\left\langle C_{p\uparrow}^{+}C_{p\uparrow}\right\rangle$ from (10) and changing the summation over p into an integration by using the relation $\sum_{p}=N(0)\int \mathrm{d}\in_p$, we obtain

$$C_{es}^{p}=\frac{2N(0)}{N}\int_0^{\hbar\omega_p}\mathrm{d}\in_p\left\{\frac{\beta\in_p\alpha_2\exp\left(\beta\alpha_2\right)}{T\left\{\exp\left(\beta\alpha_2\right)+1\right\}^2}+\frac{\beta\left(\alpha_1-\in_p\right)\in_p}{2T\sqrt{\in_p^2+\Delta_{pp}^2+\Delta_2^2+\Delta_{pp}\Delta_2^{+}+\Delta_2\Delta_{pp}^{+}}}\times\left[\frac{\alpha_1\exp\left(\beta\alpha_1\right)}{\left\{\exp\left(\beta\alpha_1\right)+1\right\}^2}-\frac{\alpha_2\exp\left(\beta\alpha_2\right)}{\left\{\exp\left(\beta\alpha_2\right)+1\right\}^2}\right]\right\} \tag{28}$$

where α_1 and α_2 are given by Equation (16).

2) For σ-band

Similarly one can write the expression for electronic specific heat C_{es}^{d} for σ-band, as

$$C_{es}^{d}=\frac{2N(0)}{N}\int_0^{\hbar\omega_d}\mathrm{d}\in_d\left\{\frac{\beta\in_d\alpha_2\exp\left(\beta\alpha_2\right)}{T\left\{\exp\left(\beta\alpha_2\right)+1\right\}^2}+\frac{\beta\left(\alpha_1-\in_d\right)\in_d}{2T\sqrt{\in_d^2+\Delta_{dd}^2+\Delta_1^2+\Delta_{dd}^{+}\Delta_1+\Delta_1^{+}\Delta_{dd}}}\times\left[\frac{\alpha_1\exp\left(\beta\alpha_1\right)}{\left\{\exp\left(\beta\alpha_1\right)+1\right\}^2}-\frac{\alpha_2\exp\left(\beta\alpha_2\right)}{\left\{\exp\left(\beta\alpha_2\right)+1\right\}^2}\right]\right\} \tag{29}$$

where α_1 and α_2 are

$$\alpha_1=+\sqrt{\in_d^2+\Delta_{dd}^2+\Delta_1^2+\Delta_{dd}^{+}\Delta_1+\Delta_1^{+}\Delta_{dd}}=+\sqrt{\in_d^2+\left(\Delta_{dd}+\Delta_1\right)^2}=+\sqrt{\in_d^2+\bar{\Delta}_d^2}$$

$$\alpha_2=-\sqrt{\in_d^2+\Delta_{dd}^2+\Delta_1^2+\Delta_{dd}^{+}\Delta_1+\Delta_1^{+}\Delta_{dd}}=-\sqrt{\in_d^2+\left(\Delta_{dd}+\Delta_1\right)^2}=-\sqrt{\in_d^2+\bar{\Delta}_d^2}$$

Electronics specific heat for π-band and σ-band are given by Equations (28) and (29) respectively.

3.3. Density of States $N(\omega)$

The density of states is an important function. This helps in the interpretation of several experimental data e.g. many processes that could occur in crystal but are forbidden because they do not conserve energy. Some of them nevertheless take place, if it is possible to correct the energy imbalance by phonon-assisted processes, which will be proportional to $N(\omega)/N(0)$ [25]. For $\omega>0$, the density of states per atom $N(\omega)$ is defined as [26,27].

$$N_p(\omega)=\lim_{\in\to 0}\frac{i}{2\pi N}\sum_{p}\left[G_{\uparrow\uparrow}\left(p,\omega+i\in\right)-G_{\uparrow\uparrow}\left(p,\omega-i\in\right)\right] \tag{30}$$

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

$$N_d(\omega)=\lim_{\in\to 0}\frac{i}{2\pi N}\sum_{d}\left[G_{\uparrow\uparrow}\left(d,\omega+i\in\right)-G_{\uparrow\uparrow}\left(d,\omega-i\in\right)\right] \tag{31}$$

where $G_{\uparrow\uparrow}$ is one particle Green function for π- and σ-bands, defined by Equations (9) and (11) respectively. We have the Green's function Equation (9),

$$\left\langle\left\langle C_{p\uparrow},C_{p\uparrow}^{+}\right\rangle\right\rangle=\frac{\left(\omega+\in_p\right)}{\left(\omega^2-E_p^2\right)} \tag{32}$$

where $E_p^2=\in_p^2+\bar{\Delta}_p^2$. Now solving Equation (32) and using partial fraction method, we obtain

$$\left\langle\left\langle C_{p\uparrow},C_{p\uparrow}^{+}\right\rangle\right\rangle=\frac{1}{2}\left[\frac{1}{\left(\omega-E_p\right)}+\frac{1}{\left(\omega+E_p\right)}\right]+\frac{\in_p}{2E_p}\left[\frac{1}{\left(\omega-E_p\right)}-\frac{1}{\left(\omega+E_p\right)}\right] \tag{33}$$

Now substituting the Green function from Equation (33) in Equation (30) and using the delta function property,

$$\underset{\in\to 0}{Lt}\frac{i}{2\pi N}\left[\frac{1}{\left(\omega+i\in-E_p\right)}-\frac{1}{\left(\omega-i\in-E_p\right)}\right]=\delta\left(\omega-E_p\right)$$

we obtain

$$N_p(\omega) = \frac{1}{2}\sum_p \left[\left(1+\frac{\in_p}{E_p}\right)\delta\left(\omega - E_p\right)+\left(1-\frac{\in_p}{E_p}\right)\delta\left(\omega + E_p\right)\right] \quad (34)$$

Changing the summation into integration and after simplification, one obtains

$$\frac{N_p(\omega)}{N_p(0)} = \begin{cases} 2\dfrac{\omega}{\sqrt{\omega^2 - \overline{\Delta}_p^2}} & \text{for } \omega > 0 \\ 0 & \text{otherwise} \end{cases} \quad (35)$$

Similarly, for σ-band

$$\frac{N_d(\omega)}{N_d(0)} = \begin{cases} 2\dfrac{\omega}{\sqrt{\omega^2 - \overline{\Delta}_p^2}} & \text{for } \omega > 0 \\ 0 & \text{otherwise} \end{cases} \quad (36)$$

4. Numerical Calculations

Values of various parameters appearing in equations obtained in the previous section are given in **Table 1**. Using these values, we study the various parameters for the system MgB_2.

4.1. Superconducting Order Parameter $\left(\overline{\Delta}\right)$

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

1) The SC order parameter for π- and σ-bands. Using Equation (25), one can write

$$\frac{V_{pd}G\left(\overline{\Delta}_d\right)}{\left[1-V_{pp}G\left(\overline{\Delta}_p\right)\right]}\times\frac{V_{pd}G\left(\overline{\Delta}_p\right)}{\left[1-V_{pp}G\left(\overline{\Delta}_d\right)\right]} = 1$$

and $\overline{\Delta} = \overline{\Delta}_p + \overline{\Delta}_d = \left(V_{pd}+V_{pp}\right)\left(G\left(\overline{\Delta}_p\right)\overline{\Delta}_p + G\left(\overline{\Delta}_d\right)\overline{\Delta}_d\right)$

Changing the variables as $\in_p = \hbar\omega_p y$, $\mathrm{d}\in_p = \hbar\omega_p \mathrm{d}y$, and taking $\mu = 0$, we obtain

Solving Equation (37) numerically, one can study the variation of superconductivity order parameters $\overline{\Delta}_p$ and $\overline{\Delta}_d$ with temperature corresponding π- and σ-bands. The behavior of superconducting order parameters corresponding to π- and σ-bands with temperature is shown in **Figure 1**.

2) SC order parameter in the presence of both π- and σ-bands.

The superconducting order parameter for combined π- and σ-bands can be studied by taking a simple sum of both the parameters. Taking the sum of order parameters $\left(\overline{\Delta} = \overline{\Delta}_\pi + \overline{\Delta}_\sigma\right)$, one can obtain the values by solving numerically. A comparison of $\overline{\Delta}$ with BCS type curve is shown in **Figure 2**.

4.2. Electronic Specific Heat (C_{es})

1) For π-band

Using Equation (28) and putting a_1, a_2 and $\beta = 1/kT$, after simplification, we obtain

$$C_{es}^p = \frac{N(0)}{2Nk_BT^2}\int_0^{\hbar\omega_p} \mathrm{d}\in_p \in_p^2 \operatorname{sech}^2\left(\frac{\sqrt{\in_p^2 + \overline{\Delta}_p^2}}{2k_BT}\right) \quad (38)$$

Changing the variables as $\in_p = \hbar\omega_p y$, $\mathrm{d}\in_p = \hbar\omega_p \mathrm{d}y$, and using parameters from **Table 1** with taking $\mu = 0$, we obtain

$$C_{es}^p = \frac{12.105\times10^{-44}}{T^2}\int_0^1 y^2\mathrm{d}y \operatorname{sech}^2\left(\frac{36.23\sqrt{2.25y^2+x^2}}{T}\right) \quad (39)$$

2) For σ-band

Similarly, we can write expression for specific heat for σ-band using Equation (29)

$$\frac{V_{pd}N_d(0)\int_0^1 \dfrac{\mathrm{d}y}{\sqrt{y^2+0.5102x^2}}\left[\dfrac{1}{\mathrm{e}^{\frac{-102}{T}\sqrt{y^2+0.5102x^2}}+1} - \dfrac{1}{\mathrm{e}^{\frac{102}{T}\sqrt{y^2+0.5102x^2}}+1}\right]}{\left[1-V_{pp}N_p(0)\int_0^1 \dfrac{\mathrm{d}y}{\sqrt{y^2+0.4444x^2}}\left[\dfrac{1}{\mathrm{e}^{\frac{-108}{T}\sqrt{y^2+0.4444x^2}}+1} - \dfrac{1}{\mathrm{e}^{\frac{108}{T}\sqrt{y^2+0.4444x^2}}+1}\right]\right]} \times \frac{V_{pd}N_p(0)\int_0^1 \dfrac{\mathrm{d}y}{\sqrt{y^2+0.4444x^2}}\left[\dfrac{1}{\mathrm{e}^{\frac{-108}{T}\sqrt{y^2+0.4444x^2}}+1} - \dfrac{1}{\mathrm{e}^{\frac{108}{T}\sqrt{y^2+0.4444x^2}}+1}\right]}{\left[1-V_{pp}N_d(0)\int_0^1 \dfrac{\mathrm{d}y}{\sqrt{y^2+0.5102x^2}}\left[\dfrac{1}{\mathrm{e}^{\frac{-102}{T}\sqrt{y^2+0.5102x^2}}+1} - \dfrac{1}{\mathrm{e}^{\frac{102}{T}\sqrt{y^2+0.5102x^2}}+1}\right]\right]} = 1 \quad (37)$$

Table 1. Values of various parameters for MgB_2 system.

S. No.	Parameter	Value	Reference
1	Superconducting transition temperature (T_c)	39 K	[1]
2	Phonon energy $(\hbar\omega_p)$ for p holes	0.00937 eV	[33]
3	Phonon energy $(\hbar\omega_p)$ for d holes	0.00875 eV	[33]
4	Density of states at the Fermi surface $N(0)$	$\cong 3.093\times10^{38}$ eV/atom	[34]
5	Pairing interaction for p holes (V_p)	$\cong 3.093\times10^{38}$ eV/atom	[18]
6	Pairing interaction for d holes (V_d)	$\cong 3.093\times10^{38}$ eV/atom	[18]
7	Pair interchange between two bands (V_{pd})	1.80 eV	[18]
8	Number of atoms per unit volume	$\sim 5\times10^{22}$	[34]
9	Crystal Structure	Hexagonal	[36]
10	Cell Parameter	$a=3.086$ Å, $c=3.524$ Å	[36]
11	Boltzmann constant (k_B)	0.00008625 eV/K	
12	Electron Mass (m_e)	9.1×10^{-31} kg	

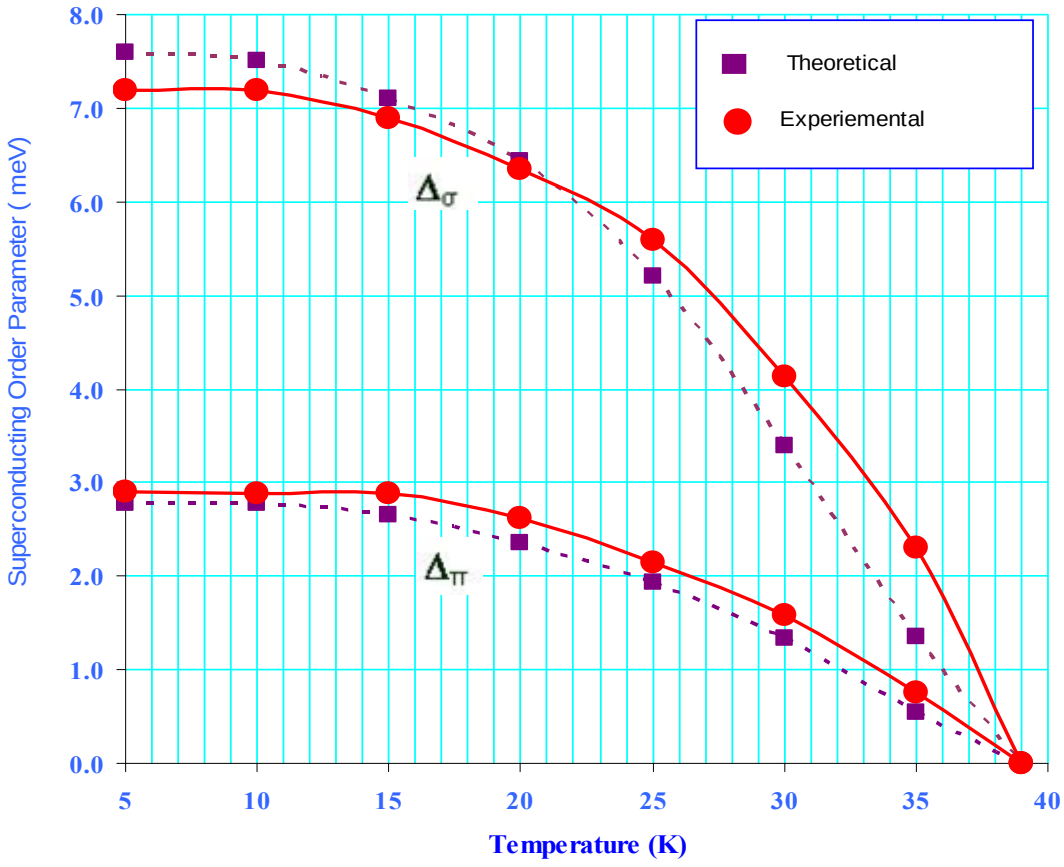

Figure 1. Variation of superconducting order parameter corresponding to π- and σ-bands with temperature [29].

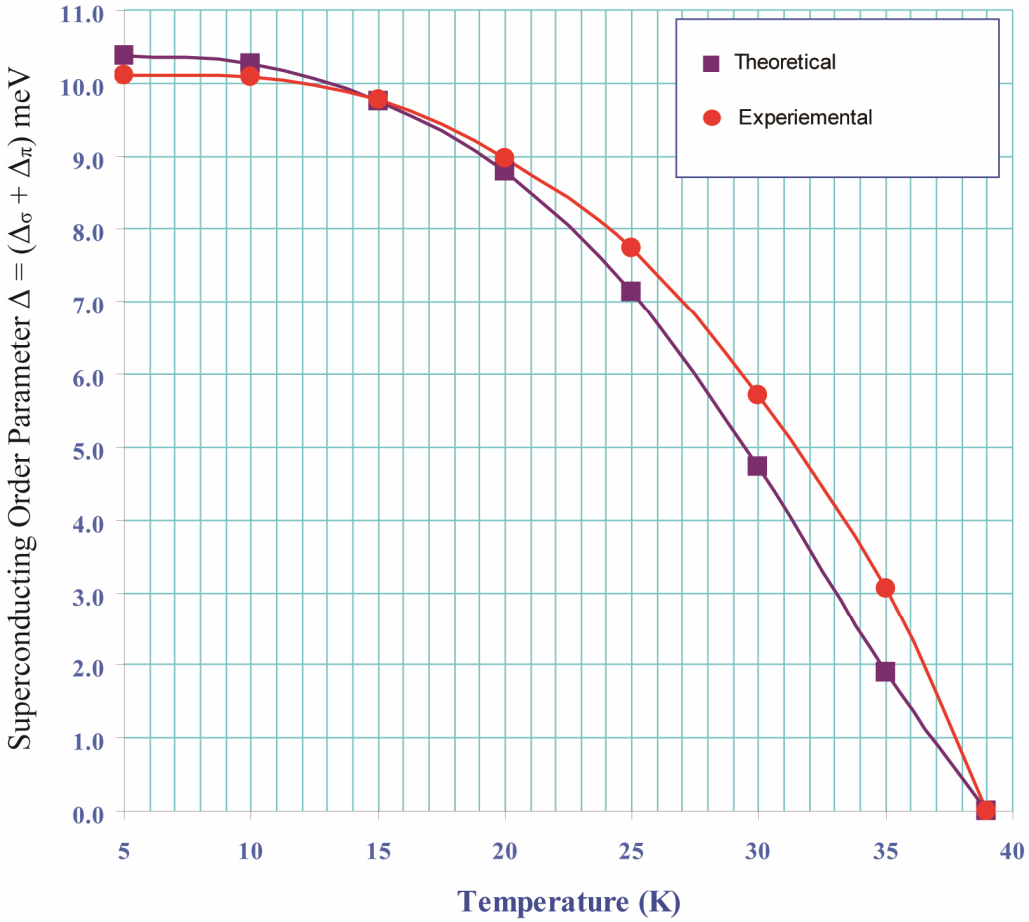

Figure 2. Variation of superconducting order parameter $\Delta = (\Delta_\pi + \Delta_\sigma)$ corresponding to π- and σ-bands with temperature.

$$C_{es}^{d} = \frac{9.841\times10^{-44}}{T^2}\int_0^1 y^2 \mathrm{d}y\,\mathrm{sech}^2\left(\frac{36.23\sqrt{1.96y^2+x^2}}{T}\right) \quad (40)$$

The variation electronic specific heat (C_{es}) with temperature (T) for π- and σ-band is shown in **Figure 3**. There is a good agreement with experiment data.

4.3. Density of States

Density of states function for the π-band is given by Equation (35). Now using the following values of y, x_1 for $\bar{\Delta}_p$ and x_2 for $\bar{\Delta}_d$, and taking $\mu = 0$, one obtains,

$$\left(\frac{N_p(\omega)}{2N_p(0)}\right) = \frac{y}{\sqrt{y^2 - x_1^2}} \quad (41)$$

Similarly, using Equation (36), density of states for σ-band is obtained as

$$\left(\frac{N_d(\omega)}{2N_d(0)}\right) = \frac{y}{\sqrt{y^2 - x_2^2}} \quad (42)$$

The above two expressions of density of states function for π- and σ-bands are similar, hence we have evaluated the values with different values of x_1 and x_2 for π- and σ-bands. The behavior of density of states function for both π- and σ-bands is shown in **Figure 4**.

5. Discussion and Conclusions

In the foregoing sections, we have presented the study of superconductivity in MgB_2 by canonical two band BCS Hamiltonian containing Fermi surfaces of π- and σ-bands. Following the Green's function technique and equation of motion method, we have obtained the expressions for superconducting order parameters $\bar{\Delta}_p$ and $\bar{\Delta}_d$, electronic specific heat, and density of states. Making use of values of various parameters given in **Table 1** for the system MgB_2, we have made study of various physical properties and wherever possible, compared our results with the available experimental data. We observe that

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

2) The temperature dependent two superconducting gaps $\bar{\Delta}_p$ and $\bar{\Delta}_d$ corresponding to π- and σ-bands for MgB_2 is found. The two gaps structure is perfectly in agreement with experimental observations [29].

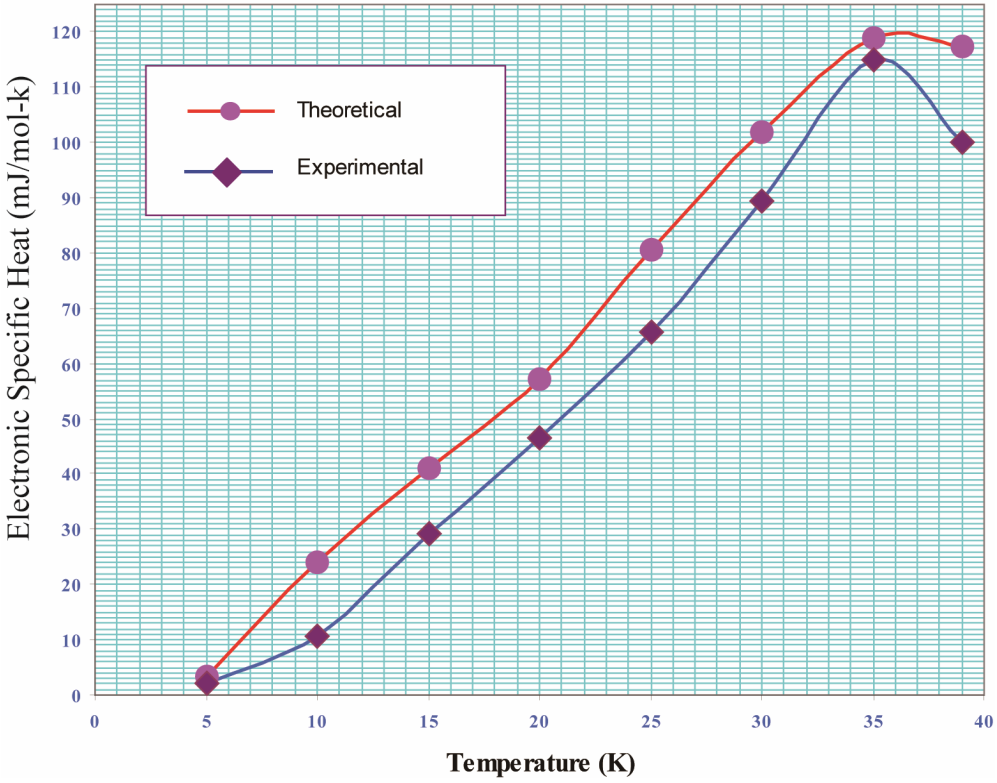

Figure 3. Variation of electronic specific heat with temperature for both π- and σ-bands.

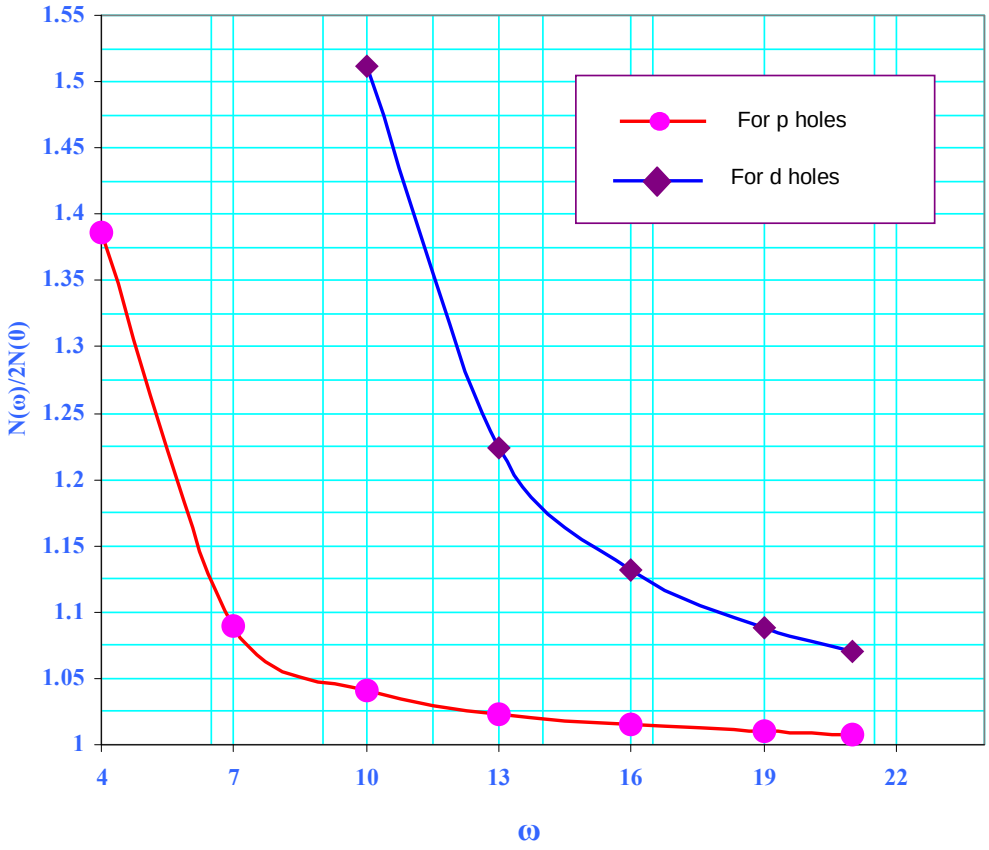

Figure 4. Variation of density of states function with ω for both π- (p holes) and σ- (d holes) bands.

3) The specific heat behaviour obtained from our model, *i.e.* C_{es} versus T is in satisfactory agreement with experimental results [30]. However, the theoretical values obtained are slightly higher than the experimental ones. This can be attributed to mean field approximations. In our model, the main interaction is V_{pd} and V_{pp} & V_{dd} are taken zero (being negligibly small). For better agreement V_{pp} and V_{dd} have to be considered. Although these interactions are very small in comparison to V_{pd}, but still they have some contribution to the specific heat of the system.

4) The density of states behaviour is similar to BCS weak coupling superconductors (**Figure 4**) corresponding to π- and σ-bands. There is marked difference between two curves. This reveals that MgB_2 superconductors differ from conventional metallic superconductors. However, the behavior of MgB_2 superconductors in this respect resembles to that of high T_c cuprates. This is a major difference between the two classes of superconductors and may be partly responsible for the difference in their properties. We may note that the density of states for the system MgB_2 is quite high [31].

Our model shows reasonable agreement with available experimental data. This mechanism emerges as a strong contender for an acceptable model for MgB_2, non cuprate high-T_c superconductor. The efforts to understand the pairing mechanism in this and other similar systems need to continue, for such efforts go hand-in-hand with enhancing future prospects for new HTSC materials and novel applications [32-35].

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