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RESEARCH ARTICLE

INVESTIGATION OF SPECIFIC HEAT, DENSITY OF STATES AND SUPERCONDUCTING GAP PARAMETERS OF MgB_2 SUPERCONDUCTOR IN TWO BAND MODELS

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ABSTRACT

The study focused on the theoretical investigation of superconducting gap parameters, density of states, electronic specific heat and condensation energy of two-band iron based superconductor MgB_2 . By developing a canonical two band BCS Hamiltonian containing a Fermi Surface of P(π)- and d(σ)-bands for the given system and by using the double time temperature dependent Green's function formalism, we obtained mathematical expressions for superconducting order parameters for the electron intra-band (Δ_p), hole intra-band (Δ_d), inter-band between the two bands (Δ_{pd}) and superconducting transition temperature (T_C). Furthermore, we obtained the density of states for each intra-band, $N(\epsilon)$, electronic specific heat (C_{es}) and condensation energy (E_c) for MgB_2 . By using the experimental values and by considering some plausible approximations of the parameters in the obtained expressions, phase diagrams of superconducting order parameters for Δ_p , Δ_d , Δ_{pd} versus temperature and superconducting transition temperature (T_C) versus the inter-band pairing potential (V_{pd}) are plotted. We also plotted the density of states for the electron intra-band, $N_p(\epsilon)$ and hole intra-band, $N_d(\epsilon)$ versus excitation energy (ϵ) at $T=0K$, and the variation of density of states with temperature, electronic specific heat for the electron intra-band (C_p) and hole intra-band (C_d) versus temperature are plotted. Similarly, phase diagrams of condensation energy (E_c) versus temperature, inter-band pairing potential and superconducting transition temperature are plotted for the material. Our results are in agreement with previous findings.

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INTRODUCTION

The surprising discovery of superconductivity in magnesium diboride (MgB_2) with transition temperature (T_C) of 39 K is the intermediate classes between low temperature and high temperature superconductors (1). Soon after the discovery scientists and technologists understood the advantages of this new intermetallic superconductor and the material got wide attention among the scientific community. MgB_2 attracted experimentalists as well as theoreticians because of its potential applications and peculiar properties which were quite unexpected in such an intermetallic. 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). Measurements of in plane and out of plane Hall coefficients show dominant hole type carriers along the a-b plane and electron type carriers along the c direction, representing the multiband nature of MgB_2 (3-5). Most of the studies pointed out that MgB_2 can be considered as a phonon-mediated BCS type superconductor, with selective coupling between specific electronic states and specific phonons are the reasons for superconductivity (6, 7, 8-11). MgB_2 is the first superconductor to show clearly two distinct superconducting gaps in its superconducting state. 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 (12-16). There is a large difference in the electron-phonon coupling on different Fermi surface sheets and this leads to multiband description of superconductivity. MgB_2 is a weak coupling two band phononic system where the Coulomb pseudo-potential and the inter-channel pairing mechanism are key terms to interpret the superconducting state (17). Coulomb potential in the d-orbitals of the transition metal reduce the isotope exponent, whereas sp-metals generally shows a nearly full isotope effect (18). It is quite natural to describe a two-gap superconductor by means of a two-band model with inter-band coupling (19,20).

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For MgB₂, 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 MgB₂ (21). We may note that two band models have been exploited in various realizations for high-T_c cuprate superconductivity (21,22). In the present study, we use σ - π inter-band coupling with a strong σ -inter-band contribution of electron-phonon and Coulomb nature. The inter-band interaction is considered to be repulsive (an advantage of two band models) corresponding to electron-electron interaction(23). Therefore I study the two-band superconductor MgB₂ has two energy gaps, Δ_p and Δ_d in the electron and hole bands respectively which vanish at the same superconducting transition temperature (T_c). The two superconducting gaps have an own intra-band “i” with coupling potential $V_{p(d)}$ in each band and the inter-band with coupling interaction potential (V_{pd}) between the two bands. The presence of inter-band pairing interaction enhances pairing of electrons and leads the superconducting gaps of the electron and hole bands to vanish at the same superconducting transition temperature (T_c) though they are different at zero temperature (24).

Theoretical Model System Hamiltonian in Two Bands

The model system Hamiltonian in the two band iron based superconductor MgB₂ is given by (24-28),

$$\hat{H} = \hat{H}_0^p + \hat{H}_0^d + \hat{H}_{pd} \quad (1)$$

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Where

$$\hat{H}_0^p = \sum_p \epsilon_p (\hat{C}_{p\uparrow}^+ \hat{C}_{p\uparrow} + \hat{C}_{-p\downarrow}^+ \hat{C}_{-p\downarrow}) - \sum_p V_{pp} (\langle \hat{C}_{p\uparrow}^+ \hat{C}_{-p\downarrow}^+ \rangle \hat{C}_{-p\downarrow} \hat{C}_{p\uparrow} + \langle \hat{C}_{p\uparrow} \hat{C}_{-p\downarrow} \rangle \hat{C}_{p\uparrow}^+ \hat{C}_{-p\downarrow}^+) \quad (2)$$

$$\hat{H}_0^d = \sum_d \epsilon_d (\hat{C}_{d\uparrow}^+ \hat{C}_{d\uparrow} + \hat{C}_{-d\downarrow}^+ \hat{C}_{-d\downarrow}) - \sum_d V_{dd} (\langle \hat{C}_{d\uparrow}^+ \hat{C}_{-d\downarrow}^+ \rangle \hat{C}_{-d\downarrow} \hat{C}_{d\uparrow} + \langle \hat{C}_{d\uparrow} \hat{C}_{-d\downarrow} \rangle \hat{C}_{d\uparrow}^+ \hat{C}_{-d\downarrow}^+) \quad (3)$$

$$\hat{H}_{pd} = \sum_{pd} V_{pd} (\langle \hat{C}_{p\uparrow}^+ \hat{C}_{-p\downarrow}^+ \rangle \hat{C}_{-d\downarrow} \hat{C}_{d\uparrow} + \langle \hat{C}_{d\uparrow} \hat{C}_{-d\downarrow} \rangle \hat{C}_{-p\downarrow} \hat{C}_{p\uparrow}) + \sum_{dp} V_{dp} (\langle \hat{C}_{d\uparrow}^+ \hat{C}_{-d\downarrow}^+ \rangle \hat{C}_{-p\downarrow} \hat{C}_{p\uparrow} + \langle \hat{C}_{p\uparrow} \hat{C}_{-p\downarrow} \rangle \hat{C}_{d\uparrow}^+ \hat{C}_{-d\downarrow}^+) \quad (4)$$

Now, substituting equations (2-4) into equation (1) we get,

$$\begin{aligned} \hat{H} = & \sum_p \epsilon_p (\hat{C}_{p\uparrow}^+ \hat{C}_{p\uparrow} + \hat{C}_{-p\downarrow}^+ \hat{C}_{-p\downarrow}) + \sum_d \epsilon_d (\hat{C}_{d\uparrow}^+ \hat{C}_{d\uparrow} + \hat{C}_{-d\downarrow}^+ \hat{C}_{-d\downarrow}) - \sum_p V_{pp} (\langle \hat{C}_{p\uparrow}^+ \hat{C}_{-p\downarrow}^+ \rangle \hat{C}_{-p\downarrow} \hat{C}_{p\uparrow} + \langle \hat{C}_{p\uparrow} \hat{C}_{-p\downarrow} \rangle \hat{C}_{p\uparrow}^+ \hat{C}_{-p\downarrow}^+) \\ & - \sum_d V_{dd} (\langle \hat{C}_{d\uparrow}^+ \hat{C}_{-d\downarrow}^+ \rangle \hat{C}_{-d\downarrow} \hat{C}_{d\uparrow} + \langle \hat{C}_{d\uparrow} \hat{C}_{-d\downarrow} \rangle \hat{C}_{d\uparrow}^+ \hat{C}_{-d\downarrow}^+) + - \sum_{pd} V_{pd} (\langle \hat{C}_{p\uparrow}^+ \hat{C}_{-p\downarrow}^+ \rangle \hat{C}_{-p\downarrow} \hat{C}_{p\uparrow} + \langle \hat{C}_{p\uparrow} \hat{C}_{-p\downarrow} \rangle \hat{C}_{p\uparrow}^+ \hat{C}_{-p\downarrow}^+) \\ & + \sum_{dp} V_{dp} (\langle \hat{C}_{d\uparrow}^+ \hat{C}_{-d\downarrow}^+ \rangle \hat{C}_{-d\downarrow} \hat{C}_{d\uparrow} + \langle \hat{C}_{d\uparrow} \hat{C}_{-d\downarrow} \rangle \hat{C}_{d\uparrow}^+ \hat{C}_{-d\downarrow}^+) \end{aligned} \quad (5)$$

Now, for

$$\begin{aligned} \Delta_{pp}^+ &= V_{pp} \langle \hat{C}_{p\uparrow}^+ \hat{C}_{-p\downarrow}^+ \rangle \\ \Delta_{dd}^+ &= V_{dd} \langle \hat{C}_{d\uparrow}^+ \hat{C}_{-d\downarrow}^+ \rangle \\ \Delta_1^+ &= V_{pd} \langle \hat{C}_{p\uparrow}^+ \hat{C}_{-p\downarrow}^+ \rangle \\ \Delta_2^+ &= V_{pd} \langle \hat{C}_{d\uparrow}^+ \hat{C}_{-d\downarrow}^+ \rangle \\ \Delta_{dd} &= V_{dd} \langle \hat{C}_{d\uparrow} \hat{C}_{-d\downarrow} \rangle \\ \Delta_1 &= V_{pd} \langle \hat{C}_{p\uparrow} \hat{C}_{-p\downarrow} \rangle \\ \Delta_2 &= V_{pd} \langle \hat{C}_{d\uparrow} \hat{C}_{-d\downarrow} \rangle \end{aligned}$$

we obtain,

$$H = \sum_p \epsilon_p (\hat{C}_{p\uparrow}^+ \hat{C}_{p\uparrow} + \hat{C}_{-p\downarrow}^+ \hat{C}_{-p\downarrow}) + \Delta_{pp}^+ \sum_p \hat{C}_{-p\downarrow} \hat{C}_{p\uparrow} + \Delta_{pp} \sum_p \hat{C}_{p\uparrow}^+ \hat{C}_{-p\downarrow}^+ + \sum_d \epsilon_d (\hat{C}_{d\uparrow}^+ \hat{C}_{d\uparrow} + \hat{C}_{-d\downarrow}^+ \hat{C}_{-d\downarrow}) + \Delta_{dd}^+ \sum_d \hat{C}_{-d\downarrow} \hat{C}_{d\uparrow} + \Delta_{dd} \sum_d \hat{C}_{d\uparrow}^+ \hat{C}_{-d\downarrow}^+ + \Delta_1^+ \sum_p \hat{C}_{-d\downarrow} \hat{C}_{d\uparrow} + \Delta_2^+ \sum_p \hat{C}_{-p\downarrow} \hat{C}_{p\uparrow} + \Delta_1 \sum_d \hat{C}_{d\uparrow}^+ \hat{C}_{-d\downarrow}^+ \quad (6)$$

where the first and second terms are the energy of conduction electrons and the terms involving superconductivity due to the intra-pairing at the electron Fermi surface respectively. The third and fourth terms are the energy of conduction electrons and the terms involving superconductivity due to the intra-pairing at the hole Fermi surface respectively. The last two terms are the terms involving superconductivity due to the inter-band between the two bands. $\hat{c}_{p\uparrow}^+$ ($\hat{c}_{-p\downarrow}$) and $\hat{c}_{d\uparrow}^+$ ($\hat{c}_{-d\downarrow}$) are the creation (annihilation) operators in the electron and hole bands respectively.

Temperature dependence of superconducting order parameters on the electron and hole in tra-bands and inter-bands: In order to find the equation of motion for the superconducting correlation function $\langle\langle \hat{c}_{p\uparrow}^+, \hat{c}_{-p\downarrow}^+ \rangle\rangle$ in the electron band, we used the double-time temperature dependent Green's function formalism (29) which is expressed as,

$$\omega \langle\langle \hat{c}_{p\uparrow}^+, \hat{c}_{-p\downarrow}^+ \rangle\rangle = \langle\langle [\hat{c}_{p\uparrow}^+, \hat{H}], \hat{c}_{-p\downarrow}^+ \rangle\rangle$$

$$\omega \langle\langle \hat{c}_{p\uparrow}^+, \hat{c}_{-p\downarrow}^+ \rangle\rangle = \langle\langle [\hat{C}_{p\uparrow}^+, \hat{H}^p] + [\hat{C}_{p\uparrow}^+, \hat{H}^d] + [\hat{C}_{p\uparrow}^+, \hat{H}^{pd}], \hat{c}_{-p\downarrow}^+ \rangle\rangle \quad (7)$$

Now, evaluating the commutating relation, $[\hat{C}_{p\uparrow}^+, \hat{H}^p]$, we obtain,

$$[\hat{C}_{p\uparrow}^+, \hat{H}^p] = (\hat{C}_{p\uparrow}^+, \sum_p \epsilon_p (\hat{C}_{p\uparrow}^+ \hat{C}_{p\uparrow} + \hat{C}_{-p\downarrow}^+ \hat{C}_{-p\downarrow})) - (\hat{C}_{p\uparrow}^+, \Delta_{pp}^+ \sum_p \hat{C}_{-p\downarrow} \hat{C}_{p\uparrow}) + (\hat{C}_{p\uparrow}^+, \Delta_{pp} \sum_p \hat{C}_{p\uparrow}^+ \hat{C}_{-p\downarrow}^+)$$

$$= \sum_p \epsilon_p ([\hat{C}_{p\uparrow}^+, \hat{C}_{p\uparrow}^+ \hat{C}_{p\uparrow}] + [\hat{C}_{p\uparrow}^+, \hat{C}_{-p\downarrow}^+ \hat{C}_{-p\downarrow}]) - \Delta_{pp}^+ \sum_p (\hat{C}_{p\uparrow}^+, \hat{C}_{-p\downarrow} \hat{C}_{p\uparrow}) + \Delta_{pp} \sum_p (\hat{C}_{p\uparrow}^+, \hat{C}_{p\uparrow}^+ \hat{C}_{-p\downarrow}^+)$$

Applying the commutations and anti-commutations rules, we have,

$$[\hat{C}_{p\uparrow}^+, \hat{H}^p] = \sum_p \epsilon_p ([\hat{C}_{p\uparrow}^+, \hat{C}_{p\uparrow}^+ \hat{C}_{p\uparrow}] + [\hat{C}_{p\uparrow}^+, \hat{C}_{-p\downarrow}^+ \hat{C}_{-p\downarrow}]) - \Delta_{pp}^+ \sum_p (\hat{C}_{p\uparrow}^+, \hat{C}_{-p\downarrow} \hat{C}_{p\uparrow}) + \Delta_{pp} \sum_p (\hat{C}_{p\uparrow}^+, \hat{C}_{p\uparrow}^+ \hat{C}_{-p\downarrow}^+)$$

From which we obtain,

$$[\hat{C}_{p\uparrow}^+, \hat{H}^p] = -\epsilon_p \hat{C}_{p\uparrow}^+ + \Delta_{pp}^+ \hat{C}_{-p\downarrow} \quad (8)$$

Furthermore, the commutating relation for $[\hat{C}_{p\uparrow}^+, \hat{H}^d]$ gives,

$$[\hat{C}_{p\uparrow}^+, \hat{H}^d] = (\hat{C}_{p\uparrow}^+, \sum_d \epsilon_d (\hat{C}_{d\uparrow}^+ \hat{C}_{d\uparrow} + \hat{C}_{-d\downarrow}^+ \hat{C}_{-d\downarrow})) - (\hat{C}_{p\uparrow}^+, \Delta_{dd}^+ \sum_d \hat{C}_{-d\downarrow} \hat{C}_{d\uparrow}) + (\hat{C}_{p\uparrow}^+, \Delta_{dd} \sum_d \hat{C}_{d\uparrow}^+ \hat{C}_{-d\downarrow}^+)$$

$$[\hat{C}_{p\uparrow}^+, \hat{H}^d] = \sum_p \epsilon_d ((\hat{C}_{p\uparrow}^+, \hat{C}_{d\uparrow}^+ \hat{C}_{d\uparrow}) + [\hat{C}_{p\uparrow}^+, \hat{C}_{-d\downarrow}^+ \hat{C}_{-d\downarrow}]) - \Delta_{dd}^+ \sum_{dd} (\hat{C}_{p\uparrow}^+, \hat{C}_{-d\downarrow} \hat{C}_{d\uparrow}) + \Delta_{dd} \sum_{dd} (\hat{C}_{p\uparrow}^+, \hat{C}_{d\uparrow}^+ \hat{C}_{-d\downarrow}^+)$$

From which we get,

$$[\hat{C}_{p\uparrow}^+, \hat{H}^d] = \quad (9)$$

Similarly, for $[\hat{C}_{p\uparrow}^+, \hat{H}^{pd}]$ we obtain,

$$[\hat{C}_{p\uparrow}^+, \hat{H}^{pd}] = \left[\hat{C}_{p\uparrow}^+, -\Delta_1^+ \sum_{pd} \hat{C}_{-d\downarrow} \hat{C}_{d\uparrow} - \Delta_2 \sum_{pd} \hat{C}_{-p\downarrow}^+ \hat{C}_{p\uparrow}^+ - \Delta_2^+ \sum_{pd} \hat{C}_{-p\downarrow} \hat{C}_{p\uparrow} - \Delta_1 \sum_{pd} \hat{C}_{d\uparrow}^+ \hat{C}_{-d\downarrow}^+ \right]$$

$$(\hat{C}_{p\uparrow}^+, \hat{H}^{pd}) = -\Delta_1^+ \sum_{pd} [\hat{C}_{p\uparrow}^+, \hat{C}_{-d\downarrow} \hat{C}_{d\uparrow}] - \Delta_2 \sum_{pd} (\hat{C}_{p\uparrow}^+, \hat{C}_{-p\downarrow}^+ \hat{C}_{p\uparrow}^+) - \Delta_2^+ \sum_{pd} (\hat{C}_{p\uparrow}^+, \hat{C}_{-p\downarrow} \hat{C}_{p\uparrow}) - \Delta_1 \sum_{pd} (\hat{C}_{p\uparrow}^+, \hat{C}_{d\uparrow}^+ \hat{C}_{-d\downarrow}^+)$$

From which we get,

$$[\hat{C}_{p\uparrow}^+, \hat{H}^{pd}] = \Delta_2^+ \hat{C}_{-d\downarrow} \quad (10)$$

Substituting equations (8-10) into equation (7), the equation of motion for $\langle\langle \hat{C}_{p\uparrow}^+, \hat{C}_{-p\downarrow}^+ \rangle\rangle$ is expressed as,

$$\langle\langle \hat{C}_{p\uparrow}^+, \hat{C}_{-p\downarrow}^+ \rangle\rangle = \frac{\Delta_{pp}^+ + \Delta_2^+}{(\omega + \epsilon_p)} \langle\langle \hat{C}_{-p\downarrow}, \hat{C}_{-p\downarrow}^+ \rangle\rangle \quad (11)$$

In the same way, the equation of motion for $\langle\langle \hat{C}_{-p\downarrow}, \hat{C}_{-p\downarrow}^+ \rangle\rangle$ becomes,

$$\omega \langle\langle \hat{C}_{-p\downarrow}, \hat{C}_{-p\downarrow}^+ \rangle\rangle = 1 + \langle\langle [\hat{C}_{-p\downarrow}, \hat{H}], \hat{C}_{-p\downarrow}^+ \rangle\rangle$$

$$\omega \langle\langle \hat{a}_{-k\downarrow}, \hat{a}_{-k\downarrow}^+ \rangle\rangle = 1 + \langle\langle [\hat{C}_{-p\downarrow}, \hat{H}] = [\hat{C}_{-p\downarrow}, \hat{H}^p] + [\hat{C}_{-p\downarrow}, \hat{H}^d] + [\hat{C}_{-p\downarrow}, \hat{H}^{pd}], \hat{a}_{-k\downarrow}^+ \rangle\rangle \quad (12)$$

Now, evaluating the following commuting relation, that is,

$$\begin{aligned}
[\hat{C}_{-p\downarrow}, \hat{H}^p] &= \sum_p \epsilon_p [\hat{C}_{-p\downarrow}, (\hat{C}_{p\uparrow}^+ \hat{C}_{p\uparrow} + \hat{C}_{-p\downarrow}^+ \hat{C}_{-p\downarrow})] - \Delta_{pp}^+ \sum_p (\hat{C}_{-p\downarrow}, \hat{C}_{-p\downarrow} \hat{C}_{p\uparrow}) - \Delta_{pp} \sum_p (\hat{C}_{-p\downarrow}, \hat{C}_{p\uparrow}^+ \hat{C}_{-p\downarrow}^+) \\
[\hat{C}_{-p\downarrow}, \hat{H}^p] &= \sum_p \epsilon_p ([\hat{C}_{-p\downarrow}, \hat{C}_{p\uparrow}^+ \hat{C}_{p\uparrow}] + [\hat{C}_{-p\downarrow}, \hat{C}_{-p\downarrow}^+ \hat{C}_{-p\downarrow}]) - \Delta_{pp}^+ \sum_p (\hat{C}_{-p\downarrow}, \hat{C}_{-p\downarrow} \hat{C}_{p\uparrow}) - \Delta_{pp} \sum_p (\hat{C}_{-p\downarrow}, \hat{C}_{p\uparrow}^+ \hat{C}_{-p\downarrow}^+)
\end{aligned}$$

Thus we get,

$$[\hat{C}_{-p\downarrow}, \hat{H}^p] = \epsilon_p \hat{C}_{-p\downarrow} + \Delta_{pp} \hat{C}_{p\uparrow}^+ \quad (13)$$

Applying the same procedures as for the electron above, the commutating relation for $[\hat{C}_{-p\downarrow}, \hat{H}^d]$ gives,

$$\begin{aligned}
[\hat{C}_{-p\downarrow}, \hat{H}^d] &= \sum_d \epsilon_d (\hat{C}_{-p\downarrow}, (\hat{C}_{d\uparrow}^+ \hat{C}_{d\uparrow} + \hat{C}_{-d\downarrow}^+ \hat{C}_{-d\downarrow})) - \Delta_{dd}^+ \sum_d (\hat{C}_{-p\downarrow}, \hat{C}_{-d\downarrow} \hat{C}_{d\uparrow}) - \Delta_{dd} \sum_d [\hat{C}_{-p\downarrow}, \hat{C}_{d\uparrow}^+ \hat{C}_{-d\downarrow}^+] \\
[\hat{C}_{-p\downarrow}, \hat{H}^d] &= \sum_d \epsilon_d ((\hat{C}_{-p\downarrow}, \hat{C}_{d\uparrow}^+ \hat{C}_{d\uparrow}) + (\hat{C}_{-p\downarrow}, \hat{C}_{-d\downarrow}^+ \hat{C}_{-d\downarrow})) - \Delta_{dd}^+ \sum_d (\hat{C}_{-p\downarrow}, \hat{C}_{-d\downarrow} \hat{C}_{d\uparrow}) - \Delta_{dd} \sum_d [\hat{C}_{-p\downarrow}, \hat{C}_{d\uparrow}^+ \hat{C}_{-d\downarrow}^+]
\end{aligned}$$

Hence we get,

$$[\hat{C}_{-p\downarrow}, \hat{H}^d] = 0 \quad (14)$$

Similarly,

$$\begin{aligned}
[\hat{C}_{-p\downarrow}, \hat{H}_{pd}] &= \left[\hat{C}_{-p\downarrow}, -\Delta_1^+ \sum_{pd} \hat{C}_{-d\downarrow} \hat{C}_{d\uparrow} - \Delta_2 \sum_{pd} \hat{C}_{-p\downarrow}^+ \hat{C}_{p\uparrow}^+ + \Delta_2^+ \sum_{pd} \hat{C}_{-p\downarrow} \hat{C}_{p\uparrow} - \Delta_1 \sum_{pd} \hat{C}_{d\uparrow}^+ \hat{C}_{-d\downarrow}^+ \right] \\
[\hat{C}_{-p\downarrow}, \hat{H}_{pd}] &= -\Delta_1^+ \sum_{pd} (\hat{C}_{-p\downarrow}, \hat{C}_{-d\downarrow} \hat{C}_{d\uparrow}) - \Delta_2 \sum_{pd} (\hat{C}_{-p\downarrow}, \hat{C}_{-p\downarrow}^+ \hat{C}_{p\uparrow}^+) - \Delta_2^+ \sum_{pd} (\hat{C}_{-p\downarrow}, \hat{C}_{-p\downarrow} \hat{C}_{p\uparrow}) - \Delta_1 \sum_{pd} [\hat{C}_{-p\downarrow}, \hat{C}_{d\uparrow}^+ \hat{C}_{-d\downarrow}^+]
\end{aligned}$$

From which we get,

$$[\hat{C}_{-p\downarrow}, \hat{H}_{pd}] = \Delta_2 \hat{C}_{p\uparrow}^+ \quad (15)$$

Substituting equations (13-15) into equation (12), the equation of motion for $\ll \hat{C}_{-p\downarrow}, \hat{C}_{-p\downarrow}^+ \gg$ becomes,

$$\ll \hat{C}_{-p\downarrow}, \hat{C}_{-p\downarrow}^+ \gg = \frac{1}{\omega - \epsilon_p} + \frac{\Delta_{pp} + \Delta_2}{\omega - \epsilon_p} \ll \hat{C}_{p\uparrow}^+, \hat{C}_{-p\downarrow}^+ \gg \quad (16)$$

Now, substituting equation (16) into equation (11) we get,

$$\ll \hat{C}_{p\uparrow}^+, \hat{C}_{-p\downarrow}^+ \gg = \frac{\Delta_{pp} + \Delta_2}{\omega^2 - \epsilon_p^2 - (\Delta_{pp} + \Delta_2)^2} \quad (17)$$

It is a well-known fact that, the superconducting order parameter in the electron band can be related to the Green's function as,

$$\Delta_{pp}^+ = \frac{V_{pp}}{2\beta} \sum_p \ll \hat{C}_{p\uparrow}^+, \hat{C}_{-p\downarrow}^+ \gg \quad (18)$$

where $\beta = \frac{1}{k_B T}$, k_B and V_{pp} are the Boltzmann constant and the pairing potential in electron intra-band respectively.

Now, we use the expression $\omega \rightarrow i\omega_n$ and Matsubara's frequency (30), given by

$$\omega_n = \frac{(2n+1)\pi}{\beta} \quad (19)$$

Substituting equations (17) and (19) into equation (18) we get,

$$\Delta_{pp}^+ = \frac{V_{pp}\beta}{2} \sum_{p,n} \left(\frac{\Delta_{pp}^+ + \Delta_2^+}{((2n+1)\pi)^2 - \beta^2 (\epsilon_p^2 - (\Delta_{pp}^+ + \Delta_2^+)^2)} \right) \quad (20)$$

By changing the summation into integration and by introducing the density of state at the Fermi level, $N_e(0)$, and using the relation,

$$\frac{\tanh(\beta\epsilon/2)}{2\beta\epsilon} = \sum_{k,n} \frac{1}{((2n+1)\pi)^2 + (\beta\epsilon)^2} \tag{21}$$

we get,

$$\Delta_{pp}^+ = V_{pp}N_p(0) \Delta_{pp}^+ \int_0^{\hbar\omega_F} \frac{\tanh\left(\frac{\beta E_p}{2}\right)}{E_p} dE_p + V_{pd}N_d(0) \Delta_{dd}^+ \int_0^{\hbar\omega_F} \frac{\tanh\left(\frac{\beta E_d}{2}\right)}{E_d} dE_d \tag{22}$$

where $\epsilon = \sqrt{\epsilon_p^2 + (\Delta_{pp} + \Delta_{pd})^2}$ and $\epsilon' = \sqrt{\epsilon_p'^2 + (\Delta_d + \Delta_{pd})^2}$

Now, if we consider the electron intra-band only, equation (22) becomes,

$$\frac{1}{V_{pp}N_p(0)} = \int_0^{\hbar\omega_F} \frac{\tanh\left(\frac{\beta E_p}{2}\right)}{E_p} dE_p \tag{23}$$

Now, using Laplace's Transform, the integral in equation (23) yields,

$$\frac{1}{v_{pp}N_p(0)} = \int_0^{\hbar\omega_F} \frac{\tanh\left(\frac{\beta}{2}\sqrt{\epsilon_p^2 + \Delta_{pp}^2}\right)}{\sqrt{\epsilon_p^2 + \Delta_{pp}^2}} dE_p - 4\beta^2 \Delta_{pp}^+ \int_0^{\hbar\omega_F} \sum_{n=0}^{\infty} \frac{1}{(\pi(2n+1))^2 \left(1 + \left(\frac{\beta E_p}{\pi(2n+1)}\right)^2\right)^2} dE_p \tag{24}$$

Using the substitution method and rearranging, equation (24) reduces to,

$$\frac{1}{v_{pp}N_p(0)} = \ln\left(1.14 \frac{\hbar\omega_F}{k_B T}\right) - \frac{4\Delta_{pp}^2 \beta^2}{\pi^3} \sum_{n=0}^{\infty} \frac{1}{(2n+1)^3} \int_0^{\infty} \frac{1}{(1+y^2)^2} dy \tag{25}$$

where $y = \frac{\beta\epsilon_e}{\pi(2n+1)}$

Applying Zeta and Riemann zeta functions, equation (25) becomes,

$$\frac{1}{v_{pp}N_p(0)} = \ln\left(1.14 \frac{\hbar\omega_F}{k_B T}\right) - \frac{\Delta_{pp}^2}{k_B^2 T_C^2} (0.1065) \tag{26}$$

At $T = T_C$, we have,

$$\frac{1}{v_{pp}N_p(0)} = \ln\left(1.14 \frac{\hbar\omega_F}{k_B T_C}\right) \tag{27}$$

Substituting equation (27) into equation (26) and using the relation $\ln(1 - x) = -x - \frac{x^2}{2} + \dots$, we get,

$$\Delta_{pp}(T) = 3.06 k_B T_C \left(1 - \frac{T}{T_C}\right)^{\frac{1}{2}} \tag{28}$$

At low temperature, the transition temperature is expressed as,

$$T_C = 1.14 \frac{\hbar\omega_F}{k_B} \exp\left(-\frac{1}{v_{pp}N(0)_p}\right) \tag{29}$$

Thus, using equation (29) in equation (28), the expression for the superconducting order parameter, $\Delta_e(T)$ for electron intra-band becomes,

$$\Delta_{pp}(T) = 3.5 \hbar\omega_F \exp\left(-\frac{1}{v_{pp}N(0)_p}\right) \left(1 - \frac{T}{T_C}\right)^{1/2} \tag{30}$$

where $N_{pp}(0) = 3.09 \text{ (meV)}^{-1}$ and $V_{pp} = 3.09 \text{ (eV)}$ are the density of state at the Fermi level and the pairing potential for the electron intra-band respectively and $\hbar\omega_F = 8.75 \text{ meV}$ is the Debye energy.

Similarly, applying the same procedure as for the electron above, the equation of motion for the superconducting correlation functions $\langle\langle \hat{c}_{k\uparrow}^\dagger, \hat{c}_{-k\downarrow}^\dagger \rangle\rangle$ for the hole intra-band becomes,

$$\langle\langle \hat{C}_{d\uparrow}^+, \hat{C}_{-d\downarrow}^+ \rangle\rangle = \frac{\Delta_{dd}^+ \Delta_1^+}{\omega + \epsilon_d} \langle\langle \hat{c}_{-d\downarrow}, \hat{c}_{-d\downarrow}^\dagger \rangle\rangle \quad (31)$$

and

$$\langle\langle \hat{c}_{-d\downarrow}, \hat{c}_{-d\downarrow}^\dagger \rangle\rangle = \frac{1}{\omega - \epsilon_d} + \frac{\Delta_{dd}^+ \Delta_1^+}{\omega - \epsilon_d} \langle\langle \hat{C}_{d\uparrow}^+, \hat{C}_{-d\downarrow}^+ \rangle\rangle \quad (32)$$

Finally, after a couple of steps the expression for the superconducting order parameter, $\Delta_h(T)$ for hole intra-band becomes,

$$\Delta_{dd}(T) = 3.5 \hbar \omega_F \exp\left(-\frac{1}{V_d N_d(0)}\right) \left(1 - \frac{T}{T_C}\right)^{1/2} \quad (33)$$

where $N_d(0) = 3.15 \text{ (meV)}^{-1}$ and $V_d = 3.093 \times 10^{38} \text{ eV(atom)}^{-1}$ are the density of state at the Fermi level and pairing potential for the hole intra-band respectively. The superconducting order parameter for the inter-band between electron and hole bands can be related to the Green's function as,

$$\Delta_1 = \frac{V_{pd}}{4\beta} \sum_{pd} (\langle\langle \hat{C}_{p\uparrow}^+, \hat{C}_{-p\downarrow}^+ \rangle\rangle + \langle\langle \hat{C}_{d\uparrow}^+, \hat{C}_{-d\downarrow}^+ \rangle\rangle) \quad (34)$$

After a couple of steps, the expression for the superconducting order parameter, $\Delta_{eh}(T)$ due to inter-band interaction between the bands is given by,

$$\Delta_1(T) = 3.5 \hbar \omega_F \exp\left(\frac{1}{V_{pd} \sqrt{N_p(0) N_d(0)}}\right) \left(1 - \frac{T}{T_C}\right)^{1/2} \quad (35)$$

where $V_{pd} = 1.80 \text{ eV}$ and is the inter-band pairing potential between the electron and the hole bands.

Dependence of superconducting transition temperature on the inter-band pairing potential: The dependence of transition temperature on the inter-band pairing potential can be studied by coupling the two superconducting equations given by (31),

$$\Delta_p = V_p N_p(0) \Delta_p \int_0^{\hbar \omega_F} \frac{\tanh\left(\frac{\beta \epsilon}{2}\right)}{\epsilon} d\epsilon + V_{pd} N_d(0) \Delta_d \int_0^{\hbar \omega_F} \frac{\tanh\left(\frac{\beta \epsilon'}{2}\right)}{\epsilon'} d\epsilon' \quad (36)$$

and

$$\Delta_d = V_d N_d(0) \Delta_d \int_0^{\hbar \omega_F} \frac{\tanh\left(\frac{\beta \epsilon'}{2}\right)}{2\epsilon'} d\epsilon' + V_{pd} N_p(0) \Delta_p \int_0^{\hbar \omega_F} \frac{\tanh\left(\frac{\beta \epsilon}{2}\right)}{2\epsilon} d\epsilon \quad (37)$$

Let

$$F(A) = \int_0^{\hbar \omega_F} \frac{\tanh\left(\frac{\beta \epsilon}{2}\right)}{2\epsilon} d\epsilon \text{ and } F(B) = \int_0^{\hbar \omega_F} \frac{\tanh\left(\frac{\beta \epsilon'}{2}\right)}{2\epsilon'} d\epsilon' \quad (38)$$

Substituting equation (38) into equations (36) and (37) we get respectively,

$$\Delta_p = V_p N_p(0) \Delta_p F(A) + V_{pd} N_d(0) \Delta_d F(B) \quad (39)$$

and

$$\Delta_d = V_d N_d(0) \Delta_d F(B) + V_{pd} N_p(0) \Delta_p F(A) \quad (40)$$

Now, rearranging equations (39) and (40) we get respectively,

$$\Delta_p [1 - V_p N_p(0) F(A)] = V_{pd} N_d(0) \Delta_d F(B) \quad (41)$$

and

$$\Delta_p [1 - V_d N_d(0) F(B)] = V_{pd} N_p(0) \Delta_p F(A) \quad (42)$$

Now, considering the products of equations (41) and (42) and rearranging we get,

$$[1 - V_p N_p(0) F(A)] [1 - V_d N_d(0) F(B)] = V_{pd}^2 N_d(0) F(B) N_p(0) F(A) \quad (43)$$

At $T = T_C$, $\Delta_p = \Delta_d = 0$. Thus, we have $F(A) = F(B) = F(T_C)$.

Therefore, equation (43) becomes,

$$[V_{pd}^2 - V_p V_d] F^2(T_C) + \left[\frac{V_p}{N_d(0)} + \frac{V_d}{N_p(0)} \right] F(T_C) - \frac{1}{N_p(0)N_d(0)} = 0 \quad (44)$$

The solution for equation (44) can be calculated as,

$$F(T_C) = \frac{-\frac{1}{2} \left[\frac{V_p}{N_d(0)} + \frac{V_d}{N_p(0)} \right] - \sqrt{\frac{1}{4} \left(\frac{V_p}{N_d(0)} + \frac{V_d}{N_p(0)} \right)^2 + \frac{V_{pd}^2 - V_p V_d}{N_p(0)N_d(0)}}}{V_{pd}^2 - V_p V_d} \quad (45)$$

$$\text{But at } T = T_C, F(T_C) = \ln \left(1.14 \frac{\hbar \omega_F}{k_B T_C} \right).$$

Finally, the expression for T_C becomes,

$$T_C = 1.14 \frac{\hbar \omega_F}{k_B} \exp \left(\frac{-V_p N_p(0) - V_d N_d(0) - \sqrt{(V_p N_p(0) + V_d N_d(0))^2 + 4(V_{pd}^2 - V_p V_d) N_p(0) N_d(0)}}{2(V_{pd}^2 - V_p V_d) N_p(0) N_d(0)} \right) \quad (46)$$

If the intra-band interactions are missing, i.e. $V_p = V_d = 0$, the transition is solely induced by the inter-band interaction and is given by,

$$T_C = 1.14 \frac{\hbar \omega_F}{k_B} \exp \left(- \frac{1}{V_{pd} \sqrt{N_p(0) N_d(0)}} \right) \quad (47)$$

Equation (47) relates T_C to V_{pd} in the two band model mediated by the inter-band pairing interaction (32).

Thus, one can easily see that, by taking $V_p = V_d = 0$, the inter-band interaction can induce the superconducting transition temperature, T_C .

Density of states in the electron and hole intra-bands

The density of states as a function of excitation energy (ε) in the electron band is defined as (33),

$$N_p(\varepsilon) = \lim_{\epsilon_p \rightarrow 0} \frac{1}{2\pi} \sum_k [G_{\uparrow\uparrow}(k, \varepsilon + i\epsilon_p(k)) - G_{\downarrow\downarrow}(k, \varepsilon - i\epsilon_p(k))] \quad (48)$$

where $G_{\uparrow\uparrow}$ is spin quasiparticles Green function for electron band. Substituting equation (11) into equation (16), we have,

$$\langle\langle \hat{C}_{-p\downarrow}^+ \hat{C}_{-p\downarrow}^+ \rangle\rangle = \frac{\omega + \epsilon_p}{\epsilon^2 - E_p^2} \quad (49)$$

$$\text{where } E_p^2 = \epsilon_p^2 + \Delta_{pp}^2$$

Using the partial fraction method, equation (49) becomes,

$$\langle\langle \hat{C}_{-p\downarrow}^+ \hat{C}_{-p\downarrow}^+ \rangle\rangle = \frac{1}{2} \left(\frac{1}{\epsilon - E_p} \right) \left(1 + \frac{\epsilon_p}{E_p} \right) + \frac{1}{2} \left(\frac{1}{\epsilon + E_p} \right) \left(1 - \frac{\epsilon_p}{E_p} \right) \quad (50)$$

Using the definition of the Dirac-delta function, the expression for the density of states in the electron intra-band of equation (48) becomes,

$$N_p(\epsilon) = \frac{1}{2} \sum_p \left[\left(1 + \frac{\epsilon_p}{E_p} \right) \delta(\epsilon - E_p) + \left(1 - \frac{\epsilon_p}{E_p} \right) \delta(\epsilon + E_p) \right] \quad (51)$$

Now, changing the summation into integration, we get,

$$N_p(\epsilon) = N_p(0) \int_0^{\hbar \omega_F} \left(1 + \frac{\epsilon_p}{E_p} \right) \delta(\epsilon - E_p) d\epsilon_p + N_p(0) \int_0^{\hbar \omega_F} \left(1 - \frac{\epsilon_p}{E_p} \right) \delta(\epsilon + E_p) d\epsilon_p \quad (52)$$

Using the Dirac-delta integration relation, $\int_{-\infty}^{\infty} f(x) \delta(x - a) dx = f(a)$, we have,

$$N_p(\epsilon) = N_p(0) \left(\frac{2\epsilon_p}{E_p} \right) \quad (53)$$

Finally, for $\epsilon_p = \epsilon$ and $E_p^2 = \epsilon^2 - \Delta_p^2$, we get,

$$N_p(\epsilon) = \begin{cases} 2N_p(0) \frac{\epsilon}{\sqrt{\epsilon^2 - \Delta_p^2}}, & \text{for } \epsilon > \Delta_p \\ 0 & \text{for } \epsilon < \Delta_p \end{cases} \tag{54}$$

Similarly, applying the same procedure as for the electron above, the density of state in the hole intra-band becomes,

$$N_d(\epsilon) = \begin{cases} 2N_d(0) \frac{\epsilon}{\sqrt{\epsilon^2 - \Delta_d^2}}, & \text{for } \epsilon > \Delta_d \\ 0 & \text{for } \epsilon < \Delta_d \end{cases} \tag{55}$$

CC

$$C_{es}^d = \frac{2N_d(0)}{N_d(T)} \int_0^{\hbar\omega_d} d\epsilon_d \left\{ \frac{\beta\epsilon_d\alpha_2\exp(\beta\alpha_2)}{T\{\exp(\beta\alpha_2)+1\}^2} + \frac{\beta(\alpha_1-\epsilon_d)\epsilon_d}{2T\sqrt{\epsilon_d^2+\Delta_{dd}^2+\Delta_1^2+\Delta_{dd}\Delta_1^++\Delta_1\Delta_{dd}^+}} \right\} \tag{63}$$

$$\times \left[\frac{\alpha_1\exp(\beta\alpha_1)}{\{\exp(\beta\alpha_1)+1\}^2} - \frac{\alpha_2\exp(\beta\alpha_2)}{\{\exp(\beta\alpha_1)+1\}^2} \right]$$

$$\alpha_1 = +\sqrt{\epsilon_d^2 + \Delta_{dd}^2 + \Delta_1^2 + \Delta_{dd}^+\Delta_1 + \Delta_1^+\Delta_{dd}} = +\sqrt{\epsilon_d^2 + (\Delta_{dd} + \Delta_1)^2} = +\sqrt{\epsilon_d^2 + \Delta_d^2}$$

$$\alpha_2 = -\sqrt{\epsilon_d^2 + \Delta_{dd}^2 + \Delta_1^2 + \Delta_{dd}^+\Delta_1 + \Delta_1^+\Delta_{dd}} = -\sqrt{\epsilon_d^2 + (\Delta_{dd} + \Delta_1)^2} = -\sqrt{\epsilon_d^2 + \Delta_d^2}$$

Electronics specific heat for π -band and σ -band are given by Equations (4.100) and (4.101) respectively.

RESULTS AND DISCUSSION

Employing the system model Hamiltonian in two bands for superconductor MgB_2 , we obtained the expressions for the dependence of superconducting order parameters for the intra and inter-bands on temperature, dependence of superconducting transition temperature (T_c) on inter-band pairing potential (V_{pd}). Furthermore, we obtained the expressions for the dependence of density of states, $N(\epsilon)$ on excitation energy and the dependency of condensation energy (E_c) on temperature, pairing potential and superconducting transition temperature. By using equations (30), (33) and (35) and by considering plausible approximations, the phase diagrams of $\Delta_p(T)$, $\Delta_d(T)$ and $\Delta_{pd}(T)$ versus temperature are plotted for MgB_2 as shown in Fig. 1. Thus, we obtained the total superconducting order parameter in two band model as a linear sum of the intra and inter-bands for MgB_2 . Furthermore, using equation (47), the phase diagram for the variation of superconducting transition temperature with inter-band pairing potential is plotted as shown in Fig. 2 for MgB_2 .

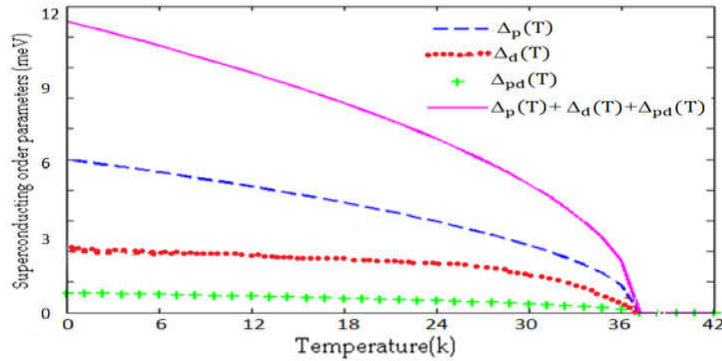


Fig. 1 Superconducting order parameters versus temperature for MgB_2

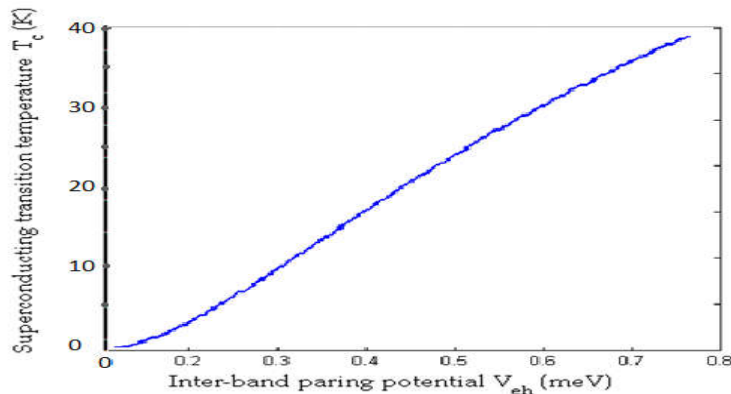


Fig. 2 Superconducting transition temperature versus inter-band pairing potential

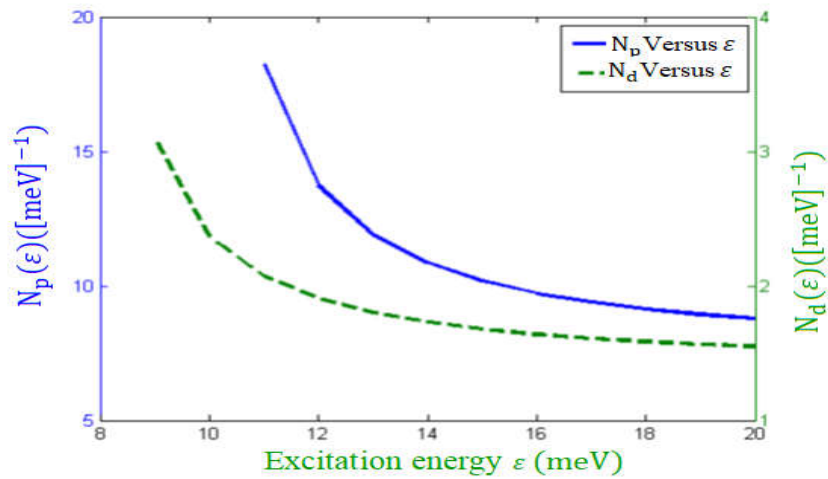


Fig. 3 Density of states for the electron and hole intra-bands at T=0K versus excitation energy for MgB₂

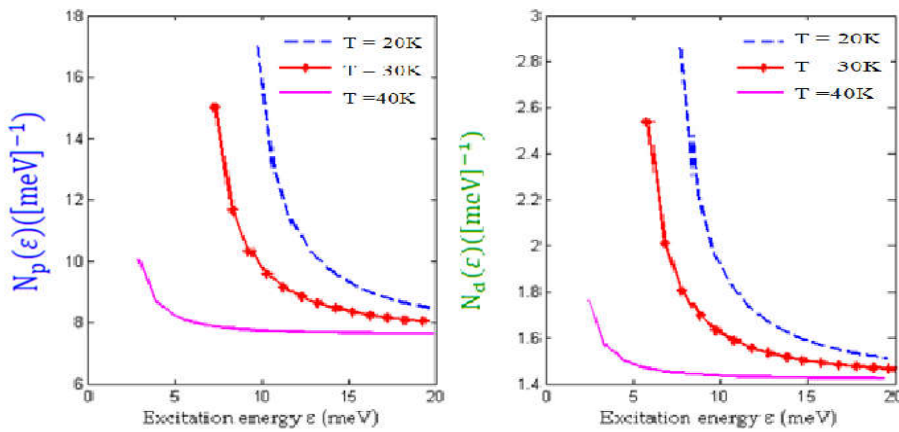


Fig. 4 Density of states for the electron and hole intra-bands at different temperatures versus excitation energy for MgB₂

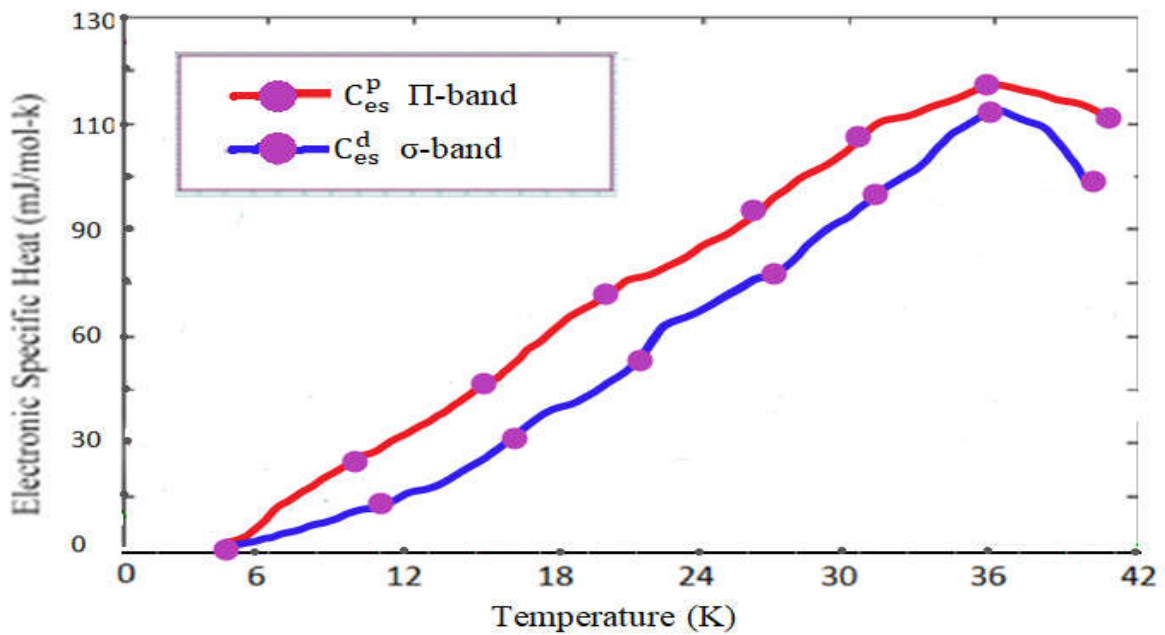


Fig. 5. Electronic specific heat for the electron and hole intra-bands versus temperatures for MgB₂

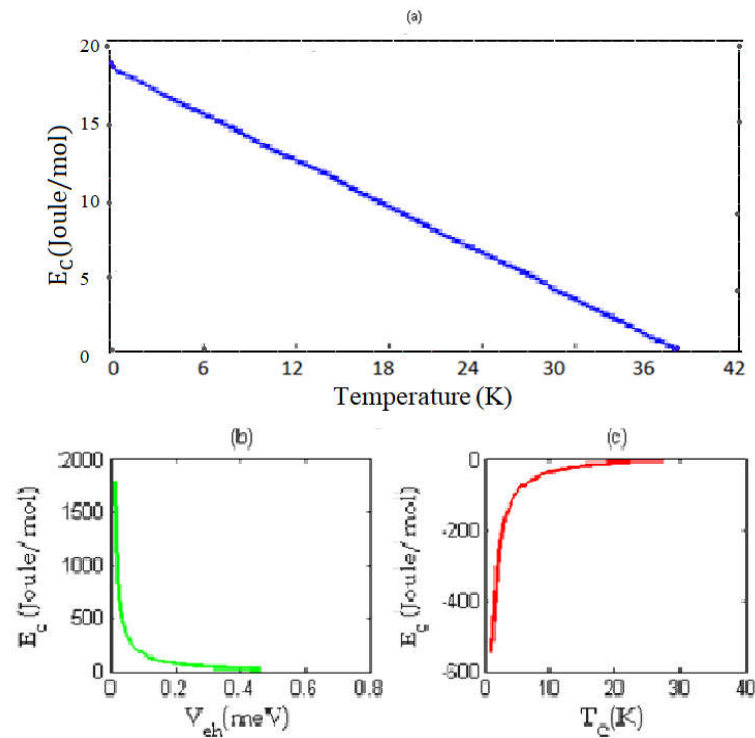


Fig.6(a) . Condensation energy versus temperature, (b) Condensation energy versus inter-band pairing potential at $T=0K$ and (c) Condensation energy versus superconducting transition temperature for MgB_2

Using equations (54) and (55), the phase diagrams for the density of states in the electron intra-band, $N_p(\epsilon)$ and hole intra-band, $N_d(\epsilon)$ versus excitation energy (ϵ) are plotted as shown in Fig. 3. Similarly, the variation of the density of states in the electron intra-band, $N_p(\epsilon)$ and hole intra-band, $N_d(\epsilon)$ with temperature are also plotted as depicted in Fig. 4. Using equations (62) and (63), the phase diagrams for the electronic specific heat in the electron intra-band, $C_p(T)$ and hole intra-band, $C_d(T)$ versus temperature are plotted as shown in Fig.5. Also, using equation (60), the phase diagrams for condensation energy versus temperature, condensation energy versus inter-band pairing potential at $T=0K$, and condensation energy versus superconducting transition temperature are plotted as shown in Figs. 6(a), 6(b) and 6(c) respectively for MgB_2 .

Conclusion

In conclusion, we have presented a two-band model by developing a model Hamiltonian for superconductor MgB_2 and using the double time temperature dependent Green's function formalism for the material which includes some of the essential concepts of the material. As shown in Fig.1, the intra and inter-band superconducting order parameters, $\Delta_p(T)$, $\Delta_d(T)$ and $\Delta_{pd}(T)$ are different at zero temperature and decrease as the temperature increases and vanish at the same superconducting transition temperature (T_c) because of the presence of inter-band pair hopping in MgB_2 . We also obtained that, the superconducting transition temperature increases with increasing inter-band pairing potential (V_{pd}) as shown in Fig. 2. As we can see from the figure, we conclude that, the two bands are not independent of each other and are coupled with each other via the inter-band pairing potential which induces pair-wise exchange between the two bands. The presence of the inter-band on one hand enhances pairing of electrons and on the other hand leads to the single superconducting transition temperature. Similarly, both the density of states for the electron and hole intra-bands vary in a similar way with the excitation energy and diverges when it approaches Δ_p and Δ_d at $T=0K$ respectively as depicted in Fig. 3. The density of states decrease with increasing temperature for each band as shown in Fig. 4. The electronic specific heat increase with increasing temperature for each band as shown in Fig. 5. Finally, the dependence of condensation energy on temperature, inter-band pairing potential and superconducting transition temperature are shown in Figs. 6(a), 6(b) and 6(c) respectively. As can be seen from Fig.6 (a) the magnitude of the condensation energy decreases with increasing temperature. Similarly, the magnitude of the condensation energy decreases with increasing inter-band pairing potential and superconducting transition temperatures as demonstrated in Figs. 6(b) and 6(c) respectively.

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