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Energy And Specific Heat Capacity Of High T_c Superconducting MgB_2 In The Two Band Model

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***Abstract*—Studies on two band superconductors have previously been described through one band model; this approach has not adequately addressed microscopic mechanisms that allow superconductivity to occur at high temperature. We reverted to canonical two band BCS Hamiltonian containing a fermi surface of p- and d- bands, followed by Bogoliubov-Valatin transformation equations, to obtain energy gap and specific heat for MgB_2 superconductor. We proposed a phonon-mediated attraction and coulomb repulsion to act differently on energy band states and stabilizing superconductor phase for MgB_2. Results were compared to the approach of a sum of two independent bands using Bardeen, Cooper and Schrieffer like π- and α-model expressions for the specific heat, entropy and free energy. We developed electron-phonon interaction model Hamiltonian for superconducting MgB_2 and its energy, obtaining expression for variation of thermodynamic properties of high Temperature superconductors in two band model system. We obtained ground state energy of 0.122264eV and Specific heat capacity as 0.1042551eV/K of MgB_2 and calculated T_C= 45.00088251K. The research demonstrated the physical and empirical meaning of the sum over the contribution of the two bands, where band parameters tend to agree with the previous determinations of band structure calculations and experiments.**

Keywords—Two-band model, Hamiltonian, Bose-Einstein Condensation, electron –phonon, cooper pair, Magnesium Diboride

1. INTRODUCTION

Mathias and Hulum (1950) pioneered the search for the high T_c superconductors in transition metal alloys and compounds. This led to independent discovery of superconductivity in thin films of the A12 compound Nb_3Ge at 23K. Superconductivity has been discovered in several other classes of materials such as the cheveral phases $A_xMO_6X_8$ that are mostly tenary transition metals chalcogenides, heavy fermion systems, organic superconductors and more recently diborides.

According to Akimitsu(Akimitsu 2001), intermetallic MgB_2 has the highest Tc at ambient pressure among all superconductors with exception of cuprates.

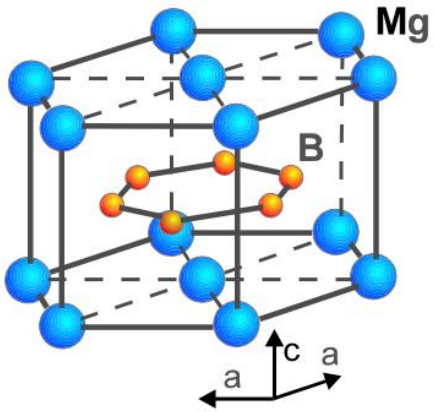

Figure 1.2 Structure containing B layers separated by hexagonal packed layers of Mg for MgB_2.

Magnesium diboride is an inorganic compound and a water-insoluble solid. It differs strikingly from most superconductors of comparable T_c, which feature transition metal. Using BCS theory and the known energy gaps of the pi and sigma bands of electrons (2.2 and 7.1 meV, respectively), the pi and sigma bands of electrons have been found to have two different coherence lengths (51 nm and 13 nm, respectively). The corresponding London penetration depths are 33.6 nm and 47.8 nm. This implies that the Ginzburg-Landau parameters are 0.66±0.02 and 3.68, respectively. The first is less than $\frac{1}{\sqrt{2}}$ and the second is greater, meaning that the first indicates marginal type I superconductivity and the second, type II superconductivity.

It has been predicted that when two different bands of electrons yield two quasiparticles, one of which has a coherence length that would indicate type I

superconductivity and one of which would indicate type II, then in certain cases, vortices attract at long distances and repel at short distances. In particular, the potential energy between vortices is minimized at a critical distance. As a consequence there is a conjectured new phase called the semi-Meissner state, in which vortices are separated by the critical distance. When the applied flux is too small for the entire superconductor to be filled with a lattice of vortices separated by the critical distance, then there are large regions of type I superconductivity, a Meissner state, separating these domains.

Experimental confirmation for this conjecture has arrived recently in MgB_2 experiments at 4.2 Kelvin. There are indeed regimes with a much greater density of vortices. Whereas the typical variation in the spacing between Abrikosov vortices in a type II superconductor is of order 1%, there is a variation of order 50%, in line with the idea that vortices assemble into domains where they may be separated by the critical distance. In our current work, we consider a two-band approach to calculating ground state energy and heat capacity of **MgB_2**.

1.1. Model Hamiltonian for two band model MgB_2 isotope.

We introduced two types of Bogoliubov quasiparticles associated with the two p and d bands of the normal pairing mechanism in each of the two separate bands as well as inter-band pairing between cooper pairs formed in different bands. According to BCS theory, a system admits a precursor phase of cooper pair triplets that undergo a phase locking transition at critical temperature. We considered a canonical two band Hamiltonian that contain a Fermi surface of p and d bands for effective Hamiltonian, which is BCS reduced Hamiltonian whose formulation is described for our system of Magnesium Diboride. We defined operators C_k^+ as creation operator for single electron state, operator C_k as destruction operator for single electron state, V_{dd} and V_{pp} as pairing interaction, V_{pd} pairing interchange between the two bands p and d and ε_k as particle energy for attractive pairing strength. We also considered two types of quasiparticles, $\left(C_{p\uparrow}C^+_{-p\downarrow}\right)$ and $C_{d\uparrow}C^+_{-d\downarrow}$ associated with the two p and d bands. The normal phonon pairing mechanism in each of the two separate bands as well as interband pairing between Cooper pairs was formed at different bands, giving effective Hamiltonian below as adopted by Thomas Thiguel (2011).

$$H = H_d + H_p + H_{\text{int}} \qquad (1.1)$$

Where H_d, H_p are given as

$$H_d = \sum_{ks} \varepsilon_{ds} C^+_{k\sigma} C_{k\sigma} + C^+_{-k\sigma} C_{-k\sigma} - \sum_{k,k^1} V_{dk^1k} C^+_{k\uparrow} C^+_{-k\downarrow} C_{k\uparrow} C_{-k^1\downarrow} + \sum_{kk^1} V_{dkk^1} C^+_{k\uparrow} C^+_{-k\downarrow} C_{k^1\uparrow} C_{-k^1\downarrow} \qquad (1.2)$$

$$H_p = \sum_{ks} \varepsilon_{p\sigma} C^+_{k\sigma} C_{k\sigma} C^+_{-k\sigma} C_{-k\sigma} - \sum_{kk^1} V_{pk^1k} C^+_{k\uparrow} C^+_{-k\downarrow} C_{k\uparrow} C_{-k\downarrow} + C_{-k^1\downarrow} C_{k\uparrow} \qquad (1.3)$$

H_d and H_p denotes free electron and interaction energy in d and p bands respectively. In equations (1.2) and (1.3), ε_{ds} *and* ε_{ps} are the kinetic energies of p and d bands, measured to relative Fermi level with spin (s) $\left(\uparrow or \downarrow\right)$, where k is the block value and V_{pkk^1} *and* V_{dkk^1} are the inter-band phonon mediated interaction matrices.

$$H_{hint} = -\sum_{k,k} V_{dpkk^1} \left(C^+_{k\uparrow} C^+_{-k\downarrow} C_{-k^1\downarrow} C_{k^1\uparrow} + C_{-k^1\downarrow} C_{k^1\uparrow} C^+_{k\uparrow} C^+_{-k\downarrow} \right) (1.4).$$

H_{hint} denote the interaction between the p and d bands and the combined form for inter-band interaction with phonon mediated matrix element V_{dpkk}^{1}.

This interaction is part of the electron interaction, here; we have ignored all other types of interaction. This turns out to be a good approximation because this interaction is the key which induces the pairs unlike other interactions that have effective energies, ie hopping effective energies.

1.2 Mean Field Approximation

In BEC, we introduced order parameter $\langle C^+ \rangle$, where the pair of electrons forms the BEC state, so that the order parameter can be written as $\sum_k \langle C^+_{k\uparrow} C^+_{-k\downarrow} \rangle$ and in condensed phase $\langle C^+_{k\uparrow} C^+_{-k\downarrow} \rangle \neq 0$ hence;

$$C^+_{k\uparrow} C^+_{-k\downarrow} = \langle C^+_{k\uparrow} C^+_{-k\downarrow} \rangle + \left(C^+_{k\uparrow} C^+_{-k\downarrow} - \langle C^+_{k\uparrow} C^+_{-k\downarrow} \rangle \right) \quad (1.5)$$

and its conjugate

$$C_{k^1\uparrow} C_{-k^1\downarrow} = \langle C_{k^1\uparrow} C_{-k\downarrow^1} \rangle + (C_{k^1\uparrow} C_{-k^1\downarrow} - \langle C_{k^1\uparrow} C_{-k^1\uparrow} \rangle) \quad (1.6)$$

We also defined X_{pd} and X^+_{pd} as

$$X^+_{pd} = \langle C^+_{k\uparrow} C^+_{-k\downarrow} \rangle \quad (1.7)$$

$$X_{pd} = \langle C_{k\uparrow} C_{-k\downarrow} \rangle \quad (1.8)$$

We defined and formulated the fluctuation term as below,

$$\sum_{k,k^1} V_{dkk^1} X^+_{pd}.X_{pd} = \sum_{kk^1} V_{pdkk^1}\left(X^+_{pd} + \left(X^+_{pd} - X^*_{pd}\right)\right)$$
$$\left(X^+_d + \left(C_{k^1\downarrow} C_{k\uparrow} - X_{pd}\right)\right) \quad (1.9)$$

After substitution, the fluctuation term was generated as below.

$$H_{Fluctuation} = \sum_{kk^1} V_{pdkk^1}\left(X^+_{pd} + \left(C^+_{k\uparrow} C^+_{-k\downarrow} - X^*_{pd}\right)\right)$$
$$\left(X^+_{pd} + \left(C_{k^1\downarrow} C_{-k\uparrow} - X_{pd}\right)\right)$$
$$= V_{pdkk^1}\left[X^+_{pd} X_{pd} + X_{pd}\right]\left(C_{k^1\downarrow} C_{-k\uparrow} - X_{pd}\right)$$
$$+ \left(C^+_{k\uparrow} C^+_{-k\downarrow} - X_{pd}\right) + very - small - factor \quad (1.11)$$

We wrote the interaction terms of the values $X_{pd} \quad and \quad X^+_{pd}$ as fluctuations. The last term of equation (1.11) is fluctuations times fluctuations. The result is too small, hence ignored. We introduced gap parameters for p and d bands respectively.

$$\Delta^+_{dd} = V_{dk} \sum_k X^*_d = V_{dkk^1} \langle C^+_{k\uparrow} C^+_{-k\downarrow} \rangle \quad (1.18)$$

$$\Delta_{dd} = C_{k^1\downarrow} C_{-k\uparrow} + V_{dd} C^+_{k\uparrow} C^+_{-k\downarrow} \quad (1.19)$$

$$\Delta^+_{pp} = V_{ppk^1} \sum_k X_k \quad (1.20)$$

$$\Delta_{pp} = V_{pkk^1} \sum_k X_p \quad (1.21)$$

Hence equations (1.2) and (1.3) are subjected to fluctuation term in equation (1.11) and gap parameters in equation (1.18),(1.19), (1.20) and (1.21)to get equation (1.22) and (1.23)

$$H_d = \sum_{ks} \varepsilon_{ds}\left(C^+_{k\uparrow} C_{k\uparrow} + \Delta^+_{dd} \sum_{k^1} C_{k^1\downarrow} C_{-k\uparrow} + \Delta_{dd} C^+_{k\uparrow} C^+_{-k\downarrow}\right) (1.22)$$

$$H_p = V_{ppk\uparrow} \sum_p \in_p u\left(C^+_{p\uparrow} C_{p\uparrow} + C^+_{-p\downarrow} C_{-p\downarrow}\right)$$
$$+ \Delta^+_{pp} \sum_p C_{-p\downarrow} C_{p\uparrow} + \Delta_{pp} \sum_p C^+_{p\uparrow} C^+_{-p\downarrow} \quad (1.23)$$

And for interaction term H_{pd}, after fluctuation operation,

$$H_{pd} = \Delta^+_1 \sum_d C_{-d\downarrow} C_{d\uparrow} + \Delta_2 \sum_p C^+_{-p\downarrow} C^+_{p\uparrow} + \Delta^+_2 \sum_p C_{-p\downarrow} C_{p\uparrow} + \Delta_1 \sum_d C^+_{d\uparrow} C^+_{-d\downarrow} (1.24)$$

The Hamiltonian for to band system of MgB_2 reduces to equation (1.25)

$$H = V_{ppk\uparrow} \sum_p \in_p u\left(C^+_{p\uparrow} C_{p\uparrow} + C^+_{-p\downarrow} C_{-p\downarrow}\right) + \Delta^+_{pp} \sum_p C_{-p\downarrow} C_{p\uparrow} + \Delta_{pp} \sum_p C^+_{p\uparrow} C^+_{-p\downarrow}$$
$$+ V_{ddk\uparrow} \sum_d \in_d u\left(C^+_{d\uparrow} C_{d\uparrow} + C^+_{-d\downarrow} C_{-d\downarrow}\right) + \Delta^+_{dd} \sum_d C_{-d\downarrow} C_{d\uparrow} + \Delta_{dd} \sum_d C^+_{d\uparrow} C^+_{-d\downarrow}$$
$$+ \Delta^+_1 \sum_d C_{-d\downarrow} C_{d\uparrow} + \Delta_2 \sum_p C^+_{-p\downarrow} C^+_{p\uparrow} + \Delta^+_2 \sum_p C_{-p\downarrow} C_{p\uparrow} + \Delta_1 \sum_d C^+_{d\uparrow} C^+_{-d\downarrow} (1.25)$$

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.

1.4 Bogoliubov-Valatin Transformation

Equation (1.25) is the adopted superfluid quadratic Hamiltonian for MgB_2 system which is diagonalized to obtain the elements of a Hamiltonian which corresponds to the stationary states when the system is in equilibrium. We described the superconducting states at T>0, and developed independently Bogoliubov-Valatin Canonical transformation equations whose description is more appropriate as follows;

The research is dealing with large number of particles, the fluctuation about the average of $\langle C_{\vec{-k}\downarrow} C^+_{\vec{k}\uparrow} \rangle$ would be small. We redefined number operators below to conform to B.V.T status as;

$$C_{\vec{-k}\downarrow} C_{\vec{k}\uparrow} = C^+\vec{k} + \left(C_{\vec{-k}\downarrow} C_{\vec{k}\uparrow} - C^+\vec{k}\right) (1.26)$$

We substitute equation (1.26) into the interaction term in equation (1.24), to get;

$$H_{pd} = \sum_{\vec{k}\sigma} V_{\vec{k}\uparrow} C^+_{\vec{k}\uparrow} C^+_{\vec{-k}\downarrow} C_{\vec{-k}\downarrow} C_{\vec{k}\uparrow} =$$
$$\sum_{\vec{k}} V_{\vec{k}}\left(C_{\vec{k}} + \left(C^+_{\vec{k}\uparrow} C^+_{\vec{-k}\downarrow} - C_{\vec{k}}\right)\right)\left(C^+_{\vec{k}} + \left(C_{\vec{-k}\downarrow} C_{\vec{k}\uparrow} - C_{\vec{k}}\right)\right)$$
$$= \sum_{\vec{k}} V_{\vec{k}}\left[\begin{array}{l} C_{\vec{k}} C^+_{\vec{k}\uparrow} C^+_{\vec{-k}} - C^+_{\vec{k}} C_{\vec{k}} C_{\vec{k}} + C_{\vec{k}} C_{\vec{-k}\downarrow} C_{\vec{-k}\uparrow} + \\ \left(C^+_{\vec{k}\uparrow} C^+_{\vec{-k}\downarrow} - C^+_{\vec{k}}\right)\left(C_{\vec{-k}} C_{\vec{k}} - C_{\vec{k}}\right) \end{array}\right] (1.27)$$

We ignore the last term on the right hand side of equation (1.27) because it's small due to large number of particles. We subject equation (1.27) to a constraint defined as;

$$u = < C_{\vec{-k}} C_{\vec{k}} >_{average} \quad (1.28)$$

We also define the parameter

$$\Delta_{\vec{k}} = \sum_{\vec{k}} V_{\vec{k}} u = -\sum_{\vec{k}} V^{+}_{\vec{k}} < C_{\vec{-k}} C_{\vec{k}} > \qquad (1.29)$$

Thus;

$$H_{pd} = +\Delta_1^{+} \sum_{d} C_{-d\downarrow} C_{d\uparrow} + \Delta_2 \sum_{p} C^{+}_{-p\downarrow} C^{+}_{p\uparrow}$$

$$+ \Delta_2^{+} \sum_{p} C^{+}_{\vec{-k}\downarrow} + \left(C_{\vec{-k}\downarrow} C_{\vec{k}\uparrow} - C^{+}_{\vec{k}\uparrow} \right) + \sum_{d} C^{+}_{d\uparrow} C^{+}_{-d\downarrow} (1.30)$$

The same operation is done on equation (1.22) and (1.23) for H_d and H_p respectively.

The total Hamiltonian after the above operations becomes bilinear form, hence diagonisable by Bogoliubov-Valatin transformation equations.

$$H = \sum_{p} \in_p \left(C^{+}_{p\uparrow} C_{p\uparrow} + C^{+}_{-p\downarrow} C_{-p\downarrow} \right)$$

$$+ \Delta_{pp}^{+} \sum_{p} C^{+}_{\vec{-k}} + \left(C_{\vec{-k}\downarrow} C_{\vec{k}\uparrow} - C^{+}_{\vec{k}\uparrow} \right) + \Delta_{pp} \sum_{p} C^{+}_{p\uparrow} C^{+}_{-p\downarrow}$$

$$+ \sum_{d} \in_d \left(C^{+}_{d\uparrow} C_{d\uparrow} + C^{+}_{-d\downarrow} C_{-d\downarrow} \right) +$$

$$\Delta_{dd}^{+} \sum_{d} C^{+}_{\vec{-k}\downarrow} + \left(C_{\vec{-k}\downarrow} C_{\vec{k}\uparrow} - C^{+}_{\vec{k}\uparrow} \right) + \Delta_{dd} \sum_{d} C^{+}_{d\uparrow} C^{+}_{-d\downarrow}$$

$$+ \Delta_1^{+} \sum_{d} C_{-d\downarrow} C_{d\uparrow} + \Delta_2 \sum_{p} C^{+}_{-p\downarrow} C^{+}_{p\uparrow}$$

$$+ \Delta_2^{+} \sum_{p} C^{+}_{\vec{-k}\downarrow} + \left(C_{\vec{-k}\downarrow} C_{\vec{k}\uparrow} - C^{+}_{\vec{k}\uparrow} \right) + \sum_{d} C^{+}_{d\uparrow} C^{+}_{-d\downarrow} (1.31)$$

Noting that the operators in equation (1.31) appear in bilinear form, they can be written in a diagonal form by appropriate transformations using C operators as shown in Bogoliubov and Valatin. We consider new operators γ and constants $u_{\vec{k}}$ *and* $v_{\vec{k}}$ which satisfy the relation;

$$\left[u_{\vec{k}} \right]^2 + \left[v_{\vec{k}} \right]^2 = 1 (1.32)$$

We also defined quasiparticles $C^{+}_{\vec{k}} C_{\vec{k}}$, $C^{+}_{\vec{-k}} C_{\vec{-k}}$, $C^{+}_{\vec{k}} C^{+}_{\vec{-k}}$ *and* $C_{\vec{-k}} C_{\vec{k}}$ separately to conform to B.V diagonalised expression as bellow,

$$C^{+}_{\vec{k}} C_{\vec{k}} = \left| u_{\vec{k}} \right|^2 \gamma^{+}_{\vec{k}} \gamma_{\vec{k}} + u_{\vec{k}} v_{\vec{k}} \gamma_{\vec{k}} \gamma_{\vec{k}} + u_{\vec{k}} \gamma_{\vec{k}} \gamma_{\vec{k}} \gamma_{\vec{k}} +$$

$$\left| u_{\vec{k}} \right|^2 \gamma_{\vec{k}} \gamma^{+}_{\vec{k}}. \quad (1.33)$$

. .

$$C^{+}_{\vec{-k}} C_{\vec{-k}} = \left| v_{\vec{k}} \right|^2 \gamma^{+}_{\vec{k}} \gamma^{+}_{\vec{k}} - u_{\vec{k}} v_{\vec{k}} \gamma^{+}_{\vec{k}}$$

$$- u_{\vec{k}} v_{\vec{k}} \gamma_{\vec{k}} \gamma_{\vec{k}} + \left| v_{\vec{k}} \right|^2 \gamma^{+}_{\vec{k}} \gamma_{\vec{k}} \qquad (1.34)$$

Similarly

$$C^{+}_{\vec{k}} C^{+}_{\vec{-k}} = u_{\vec{k}} v_{\vec{k}} \gamma^{+}_{\vec{k}} \gamma_{\vec{k}} - \left| v_{\vec{k}} \right|^2 \gamma_{\vec{k}} \gamma_{\vec{k}} + .$$

$$u^2_{\vec{k}} \gamma^{+}_{\vec{k}} \gamma^{+}_{\vec{k}} + u_{\vec{k}} v_{\vec{k}} \gamma_{\vec{k}} \gamma^{+}_{\vec{k}}. (1.35)$$

$$C_{\vec{-k}} C_{\vec{k}} = -v_{\vec{k}} u_{\vec{k}} \gamma^{+}_{\vec{k}} \gamma_{\vec{k}} + \left| u_{\vec{k}} \right|^2 \gamma_{\vec{k}} \gamma_{\vec{k}} -$$

$$\left| v_{\vec{k}} \right|^2 \gamma^{+}_{\vec{k}} \gamma^{+}_{\vec{k}} + u_{\vec{k}} v_{\vec{k}} \gamma_{\vec{k}} \gamma_{\vec{k}} \gamma^{+}_{\vec{k}}. \quad (1.36)$$

We now substitute equations (1.34), (1.35), and (1.36), into equation (1.22.), (1.23) and (1.24) for H_p, H_d and H_{pd} respectively. When the coefficients of $\gamma_{\vec{k}} \gamma_{\vec{k}}$ *and* $\gamma^{+}_{\vec{k}} \gamma^{+}_{\vec{k}}$ vanish and we collect like terms together, we obtain;

$$H_d = \in_d \left(\begin{array}{l} \left| u_{\vec{k}} \right|^2 \gamma^{+}_{\vec{k}} \gamma_{\vec{k}} + \gamma_{\vec{k}} \gamma_{\vec{k}} + \left| v_{\vec{k}} \right|^2 \gamma_{\vec{k}} \gamma^{+}_{\vec{k}} + \gamma^{+}_{\vec{k}} \gamma^{+}_{\vec{k}} - \\ u_{\vec{k}} v_{\vec{k}} \gamma_{\vec{k}} + \left| v_{\vec{k}} \right|^2 \gamma^{+}_{\vec{k}} \gamma_{\vec{k}} \end{array} \right)$$

$$+ \Delta_{dd}^{+} \sum_{d} \gamma^{+}_{\vec{k}} + \left(\begin{array}{l} - v_{\vec{k}} u_{\vec{k}} \gamma^{+}_{\vec{k}} \gamma_{\vec{k}} + \gamma_{\vec{k}} \gamma_{\vec{k}} - \gamma^{+}_{\vec{k}} \gamma^{+}_{\vec{k}} + \\ u_{\vec{k}} v_{\vec{k}} \gamma_{\vec{k}} \gamma_{\vec{k}} \gamma^{+}_{\vec{k}} + v_{\vec{k}} \gamma_{\vec{k}} \gamma_{\vec{k}} + u_{\vec{k}} \gamma^{+}_{\vec{k}} \end{array} \right) +$$

$$\Delta_{dd} \sum_{d} u_{\vec{k}} v_{\vec{k}} \gamma^{+}_{\vec{k}} - \gamma_{\vec{k}} \gamma_{\vec{k}} + \gamma^{+}_{\vec{k}} \gamma^{+}_{\vec{k}} + u_{\vec{k}} v_{\vec{k}} \gamma_{\vec{k}} \gamma^{+}_{\vec{k}}. \quad (1.37)$$

$$H_p = \in_p \sum_p \begin{pmatrix} \left|u_{\vec{k}}\right|^2 \gamma^+_{\vec{k}}\gamma_{\vec{k}} + \gamma_{\vec{k}}\gamma_{\vec{k}} + \left|v_{\vec{k}}\right|^2 \gamma_{\vec{k}}\gamma^+_{\vec{k}} \\ + \gamma^+_{\vec{k}}\gamma^+_{\vec{k}} - u_{\vec{k}}v_{\vec{k}}\gamma_{\vec{k}} + \left|v_{\vec{k}}\right|^2 \gamma^+_{\vec{k}}\gamma_{\vec{k}} \end{pmatrix}$$

$$+ \Delta^+_{pp}\sum_p \gamma^+_{\vec{k}} + \begin{pmatrix} -v_{\vec{k}}u_{\vec{k}}\gamma^+_{\vec{k}}\gamma_{\vec{k}} + \gamma_{\vec{k}}\gamma_{\vec{k}} - \gamma^+_{\vec{k}}\gamma^+_{\vec{k}} \\ + u_{\vec{k}}v_{\vec{k}}\gamma_{\vec{k}}\gamma_{\vec{k}}\gamma^+_{\vec{k}} + v_{\vec{k}}\gamma_{\vec{k}} + u_{\vec{k}}\gamma^+_{\vec{k}} \end{pmatrix}$$

$$\Delta_{pp}\sum_d u_{\vec{k}}v_{\vec{k}}\gamma^+_{\vec{k}} - \gamma_{\vec{k}}\gamma_{\vec{k}} + \gamma^+_{\vec{k}}\gamma^+_{\vec{k}} + u_{\vec{k}}v_{\vec{k}}\gamma_{\vec{k}}\gamma^+_{\vec{k}} \quad (1.38)$$

$$H_{pd} = \Delta^+_1 \sum_d \left(-v_{\vec{k}}u_{\vec{k}}\gamma^+_{\vec{k}}\gamma_{\vec{k}} + \gamma_{\vec{k}}\gamma_{\vec{k}} + u_{\vec{k}}v_{\vec{k}}\gamma_{\vec{k}}\gamma_{\vec{k}}\gamma^+_{\vec{k}}\right)$$
$$+ \Delta_2 \sum_p u_{\vec{k}}v_{\vec{k}}\gamma^+_{\vec{k}} - \gamma_{\vec{k}}\gamma_{\vec{k}} + \gamma^+_{\vec{k}}\gamma^+_{\vec{k}} + u_{\vec{k}}v_{\vec{k}}\gamma_{\vec{k}}\gamma^+_{\vec{k}}$$
$$+ \Delta^+_2 \sum_p -v_{\vec{k}}\gamma_{\vec{k}} + u_{\vec{k}}\gamma^+_{\vec{k}}$$
$$+ \left(-v_{\vec{k}}u_{\vec{k}}\gamma^+_{\vec{k}}\gamma_{\vec{k}} + u_{\vec{k}}v_{\vec{k}}\gamma_{\vec{k}}\gamma_{\vec{k}}\gamma^+_{\vec{k}} + v_{\vec{k}}\gamma_{\vec{k}} + u_{\vec{k}}\gamma^+_{\vec{k}}\right)$$
$$+ u_{\vec{k}}v_{\vec{k}}\gamma^+_{\vec{k}}\gamma_{\vec{k}} - \gamma_{\vec{k}}\gamma_{\vec{k}} + \gamma^+_{\vec{k}}\gamma^+_{\vec{k}} + u_{\vec{k}}v_{\vec{k}}\gamma_{\vec{k}}\gamma^+_{\vec{k}} \quad (1.39)$$

Putting all terms together in equations (1.37),(1.38) and (1.39) , the model Hamiltonian for magnesium diBoride for phonon-mediated attraction and coulomb repulsion reduces to ;

$$H_M = \varepsilon_p \gamma^+_{\vec{k}}\gamma^+_{\vec{k}}\gamma_{\vec{k}}\gamma_{\vec{k}} - \gamma_{\vec{k}}\gamma_{\vec{k}} + \varepsilon_d \gamma^+_{\vec{k}}\gamma_{\vec{k}}\gamma^+_{\vec{k}}\gamma_{\vec{k}}$$
$$+ v_{pd}\gamma_{\vec{k}}\gamma_{\vec{k}}\gamma^+_{\vec{k}}\gamma_{\vec{k}}\gamma_{\vec{k}}\gamma^+_{\vec{k}}\gamma^+_{\vec{k}}$$
$$+ \gamma^+_{\vec{k}}\gamma^+_{\vec{k}} + \gamma_{\vec{k}}\gamma_{\vec{k}} + \Delta^+_{pd}u_{\vec{k}}\gamma_{\vec{k}}\gamma_{\vec{k}} - v_{\vec{k}}\gamma^+_{\vec{k}}\gamma^+_{\vec{k}}\gamma^+_{\vec{k}}\gamma_{\vec{k}}\gamma_{\vec{k}}\gamma_{\vec{k}} \quad (1.40)$$

The operators obey the bosonic anti-commutation relationships as per equation below

$$\left[\gamma^+_{\vec{k}}, \gamma\right]_+ = \delta_{\vec{k}} \quad (1.41)$$

Hence equation (1.40) reduces to;

$$H_M = \varepsilon_p \gamma^+_{\vec{k}}\gamma^+_{\vec{k}}\gamma_{\vec{k}}\gamma_{\vec{k}} + \varepsilon_d \gamma^+_{\vec{k}}\gamma_{\vec{k}}\gamma^+_{\vec{k}}\gamma_{\vec{k}}$$
$$+ \gamma_{\vec{k}}\gamma_{\vec{k}}\gamma^+_{\vec{k}}\gamma_{\vec{k}}\gamma_{\vec{k}}\gamma^+_{\vec{k}}\gamma^+_{\vec{k}} + \Delta^+_{pd}u_{\vec{k}}\gamma_{\vec{k}}\gamma_{\vec{k}}\gamma^+_{\vec{k}}$$
$$- v_{\vec{k}}\gamma^+_{\vec{k}}\gamma^+_{\vec{k}}\gamma^+_{\vec{k}}\gamma_{\vec{k}}\gamma_{\vec{k}}\gamma_{\vec{k}} \quad (1.42)$$

Then model Hamiltonian in (1.42) is the diagonalized equation by Bogoliubov-Valatin transformation equations.

2.6 Ground state energy

We now calculate the energy that is required during the interaction using the normalized wave function Ψ.

$$E_n = \langle\Psi|H_M|\psi\rangle$$
$$\langle\Psi|H_M|\Psi\rangle = \langle 0|\varepsilon_p \gamma^+_{\vec{k}}\gamma^+_{\vec{k}}\gamma_{\vec{k}}\gamma_{\vec{k}} + \varepsilon_p \gamma^+_{\vec{k}}\gamma_{\vec{k}}\gamma^+_{\vec{k}}\gamma_{\vec{k}}$$
$$+ \gamma_{\vec{k}}\gamma_{\vec{k}}\gamma^+_{\vec{k}}\gamma_{\vec{k}}\gamma_{\vec{k}}\gamma^+_{\vec{k}}\gamma^+_{\vec{k}}$$
$$+ \Delta^+_{pd}u_{\vec{k}}\gamma_{\vec{k}}\gamma_{\vec{k}}\gamma^+_{\vec{k}} - v_{\vec{k}}\gamma^+_{\vec{k}}\gamma^+_{\vec{k}}\gamma^+_{\vec{k}}\gamma_{\vec{k}}\gamma_{\vec{k}}\gamma_{\vec{k}}|0\rangle \quad (1.43)$$

Where the vacuum state is represented by $|0\rangle$ has three distinct spaces i.e $|0\rangle = |0_{-k} \quad ,0_k \quad ,0_{k^1}\rangle$ (1.44)

By doing expansion on terms in the equation and performing the bra-ket operation on each term in the bra-ket, followed by factorization, we set equation (1.44) for normalization case by rewriting it as in equation (1.45)

$$E_g = \langle 0|u_{\vec{k}}\gamma^+_{\vec{k}}\varepsilon_p \gamma^+_{\vec{k}}\gamma^+_{\vec{k}}\gamma_{\vec{k}}\gamma_{\vec{k}}v_{\vec{k}}\gamma_{\vec{k}}|0\rangle$$
$$+ \langle 0|u_{\vec{k}}\gamma^+_{\vec{k}}\varepsilon_p \gamma^+_{\vec{k}}\gamma_{\vec{k}}\gamma^+_{\vec{k}}\gamma_{\vec{k}}v_{\vec{k}}\gamma_{\vec{k}}|0\rangle$$
$$+ \langle 0|u_{\vec{k}}\gamma^+_{\vec{k}}\gamma_{\vec{k}}\gamma_{\vec{k}}\gamma^+_{\vec{k}}\gamma_{\vec{k}}\gamma_{\vec{k}}\gamma^+_{\vec{k}}\gamma^+_{\vec{k}}v_{\vec{k}}\gamma_{\vec{k}}|0\rangle$$
$$+ \langle 0|u_{\vec{k}}\gamma^+_{\vec{k}}\Delta^+_{pd}u_{\vec{k}}\gamma_{\vec{k}}\gamma_{\vec{k}}\gamma^+_{\vec{k}}v_{\vec{k}}\gamma_{\vec{k}}|0\rangle$$
$$- \langle 0|u_{\vec{k}}\gamma^+_{\vec{k}}v_{\vec{k}}\gamma^+_{\vec{k}}\gamma^+_{\vec{k}}\gamma^+_{\vec{k}}\gamma_{\vec{k}}\gamma_{\vec{k}}\gamma_{\vec{k}}v_{\vec{k}}\gamma_{\vec{k}}|0\rangle \quad (1.45)$$

Hence we rewrite equation (1.45) as

$$E_g = \langle 0_k 0_{-k} 0_{k^1}|u_{\vec{k}}\gamma^+_{\vec{k}}\varepsilon_p \gamma^+_{\vec{k}}\gamma^+_{\vec{k}}\gamma_{\vec{k}}\gamma_{\vec{k}}v_{\vec{k}}\gamma_{\vec{k}}|0_k 0_{-k} 0_{k^1}\rangle$$
$$+ \langle 0_k 0_{-k} 0_{k^1}|u_{\vec{k}}\gamma^+_{\vec{k}}\varepsilon_p \gamma^+_{\vec{k}}\gamma_{\vec{k}}\gamma^+_{\vec{k}}\gamma_{\vec{k}}v_{\vec{k}}\gamma_{\vec{k}}|0_k 0_{-k} 0_{k^1}\rangle$$
$$+ \langle 0_k 0_{-k} 0_{k^1}|u_{\vec{k}}\gamma^+_{\vec{k}}\gamma_{\vec{k}}\gamma_{\vec{k}}\gamma^+_{\vec{k}}\gamma_{\vec{k}}\gamma_{\vec{k}}\gamma^+_{\vec{k}}\gamma^+_{\vec{k}}v_{\vec{k}}\gamma_{\vec{k}}|0_k 0_{-k} 0_{k^1}\rangle$$
$$+ \langle 0_k 0_{-k} 0_{k^1}|u_{\vec{k}}\gamma^+_{\vec{k}}\Delta^+_{pd}u_{\vec{k}}\gamma_{\vec{k}}\gamma_{\vec{k}}\gamma^+_{\vec{k}}v_{\vec{k}}\gamma_{\vec{k}}|0_k 0_{-k} 0_{k^1}\rangle$$
$$- \langle 0_k 0_{-k} 0_{k^1}|u_{\vec{k}}\gamma^+_{\vec{k}}v_{\vec{k}}\gamma^+_{\vec{k}}\gamma^+_{\vec{k}}\gamma^+_{\vec{k}}\gamma_{\vec{k}}\gamma_{\vec{k}}\gamma_{\vec{k}}v_{\vec{k}}\gamma_{\vec{k}}|0_k 0_{-k} 0_{k^1}\rangle \quad (1.46)$$

Noting that $\gamma^+|0\rangle = |1\rangle, \quad \gamma|0\rangle = 0, \quad and \quad \gamma|1\rangle = |0\rangle$, then equation (1.46) is simplified to;

$$E_g = \varepsilon_p v_{\underset{k}{\rightarrow}}^2 + \varepsilon_d u_{\underset{k}{\rightarrow}}^2 + 0 + \Delta_{\underset{k}{\rightarrow}}^+ u_{\underset{k}{\rightarrow}}^2 v_{\underset{k}{\rightarrow}} - v_{\underset{k}{\rightarrow}}^2 u_{\underset{k}{\rightarrow}} \quad (1.47)$$

$$E_g = \varepsilon_p v_{\underset{k}{\rightarrow}}^2 + \varepsilon_d u_{\underset{k}{\rightarrow}}^2 + \Delta_{\underset{k}{\rightarrow}}^+ u_{\underset{k}{\rightarrow}}^2 v_{\underset{k}{\rightarrow}} - v_{\underset{k}{\rightarrow}}^2 u_{\underset{k}{\rightarrow}} \quad (1.48)$$

If $\varepsilon_p = \varepsilon_d = \varepsilon_{pd}$ (1.49)

then

$$E_g = \varepsilon_{pd} + \Delta_{\underset{k}{\rightarrow}}^+ u_{\underset{k}{\rightarrow}}^2 v_{\underset{k}{\rightarrow}} - v_{\underset{k}{\rightarrow}}^2 u_{\underset{k}{\rightarrow}} \quad (1.50)$$

Equation (1.50) is the ground state energy of two band model, the case of magnesium diBoride. It differs from energy of one band model due the additional $\varepsilon_{pd} + \Delta_{\underset{k}{\rightarrow}}^+$ terms of energy showing the lowest energy achieved in the p and d bands at vacuum state, indicating formation of the bands at lowest energy in the system.

The two band model possess lower energy at vacuum state compared to one band model superconductor, hence bosons can be formed at lowest energy of magnesium diboride. In relating the above energy with temperature, we multiply equation (1.50) with thermal activation factor.

So that;

$$E_n = E_g e^{-E_g/100k_BT} \quad (1.52)$$

Therefore the energy of the system of magnesium diBoride at any temperature T is given as ;

$$E_n = \left(\varepsilon_{pd} + \Delta_k^+ u_k^2 v_k - v_k^2 u_k\right) e^{-\left(\varepsilon_{pd} + \Delta_k^+ u_k^2 v_k - v_k^2 u_k\right)/100k_BT} \quad (1.53)$$

2.7 Specific heat capacity.

We now obtain the expression for specific heat capacity of the two band system for magnesium diBoride. As a standard procedure, specific heat capacity of a system at constant volume is obtained from the temperature derivative of energy of the system.

$$C_V = \frac{dE_n}{dT} \quad (1.54)$$

We introduce

$$\beta = \left(\varepsilon_{pd} + \Delta_k^+ u_k^2 v_k - v_k^2 u_k\right)/100k_B \quad (1.55)$$

And substitute equation (1.55) into equation (1.54) to get ;

$$E_n = \left(\varepsilon_{pd} + \Delta_k^+ u_k^2 v_k - v_k^2 u_k\right) e^{\beta/T} \quad (1.56)$$

We let $t = \frac{\beta}{T}$

Therefore

$$E_n = \left(\varepsilon_{pd} + \Delta_k^+ u_k^2 v_k - v_k^2 u_k\right) e^t \quad (1.57)$$

Or $E_n = E_g e^t$

$$C_V = \frac{d\left(\varepsilon_{pd} + \Delta_k^+ u_k^2 v_k - v_k^2 u_k\right)/e^t}{dT}$$

$$but \quad dt = \frac{-\beta}{T^2} dT$$

$$C_V = \frac{d}{\frac{-T^2}{\beta} dt} \left(\varepsilon_{pd} + \Delta_k^+ u_k^2 v_k - v_k^2 u_k\right) e^t$$

$$C_V = \frac{\beta\left(\varepsilon_{pd} + \Delta_k^+ u_k^2 v_k - v_k^2 u_k\right)}{T^2} e^t$$

$$C_V = \frac{\left(\varepsilon_{pd} + \Delta_k^+ u_k^2 v_k - v_k^2 u_k\right)^2}{k_B T^2} e^{-\left(\varepsilon_{pd} + \Delta_k^+ u_k^2 v_k - v_k^2 u_k\right)/100k_BT} \quad (1.59)$$

The equation (1.59) is the specific heat formula.

2.8 Electronic specific heat (Ces)

The electronic specific heat is heat perelectron of a superconductor and it is determined from the relation

(For p bands);

$$C_{es}^p = \frac{\partial}{\partial T} \frac{1}{N} \sum_p 2\left(\in_p - \mu\right) \langle C_{p\uparrow}^+ C_{p\uparrow} \rangle \quad (1.60)$$

Where $\in$ is the energy of pi band and u is the common chemical potential. Substituting $\langle C_{p\uparrow}^+ C_{p\uparrow} \rangle$ and changing the summation over p into an integration by using the relation $\sum_p = N\left(0 \int d \in_p\right)$ we obtained;

$$C_{es}^p = \frac{2N(0)}{N} \int_0^{\hbar\omega_p} d \in_p \left\{ \frac{\beta \in_p \alpha_2 \exp(\beta\alpha_2)}{T\{\exp(\beta\alpha_2)+1\}^2} + \frac{\beta\left(\alpha - \in_1 - \in_p\right)}{2T\sqrt{\in_p^2 + \Delta_{pp}^2 + \Delta_2^2 + \Delta_{pp}\Delta_2^+ + \Delta_2\Delta_{pp}^+}} \right\} (1.61)$$

Using the above equation after simplification and replacing $\beta = \frac{-1}{kT}$, we obtained

$$C_{es}^{p} = \frac{N(0)}{2NK_B T^2}\int_0^{\hbar\omega_p} d\in_p \in_p^2 \sec h^2\left(\frac{\sqrt{\in_p^2 + \sqrt{\Delta_p^2}}}{2K_B T}\right) \quad (1.62)$$

Changing the phonon energy variables as $\in_p = \hbar\omega_p y, d\in_p = \hbar\omega_p dy$ and taking $\mu = 0$, we obtain

$$C_{es}^{p} = \frac{12.105x10^{-44}}{T^2}\int_0^1 y^2 dy \sec h^2\left(\frac{36.25\sqrt{2.25y^2 + x^2}}{T}\right) (1.63)$$

For sigma band, we write the expression;

$$C_{es}^{d} = \frac{9.84x10^{-44}}{T^2}\int_0^1 y^2 \sec h^2\left(\frac{36.23\sqrt{1.96y^2 + x^2}}{T}\right)$$

$$C_{es}^{d} = \frac{1.2105x10^{-43}}{T^2}.\frac{1}{3}.\sec h^2\left(\frac{36.25\sqrt{2.25y^2 + x^2}}{T}\right)$$

$$C_{es}^{d} = \frac{4.388x10^{-42}}{3T^3}.\frac{\sqrt{2.25(26.7)^2 + 0.0667^2}}{\cos 4.304x10^{-67}}$$

$$C_{es}^{d} = \frac{1.1722x10^{-41}}{3T^3}$$

$$C_{es}^{d} = \frac{3.9703x10^{-42}}{T^3} \quad (1.64)$$

The variation of electronic specific heat with temperature (T) for pi and sigma bands is shown with good agreement with experimental data.

Using the above equation and putting $\beta = {}^{1}/_{kT}$ after simplification, we obtain

$$C_{es}^{b} = \frac{12.105x10^{-44}}{T^2}\int_0^1 y^2 dy \sec h^2\left(\frac{36.23\sqrt{2.25y^2 + x^2}}{T}\right) \quad (1.64)$$

2.9 Results and discussion

2.9.1 Variation of electronic specific heat with temperature

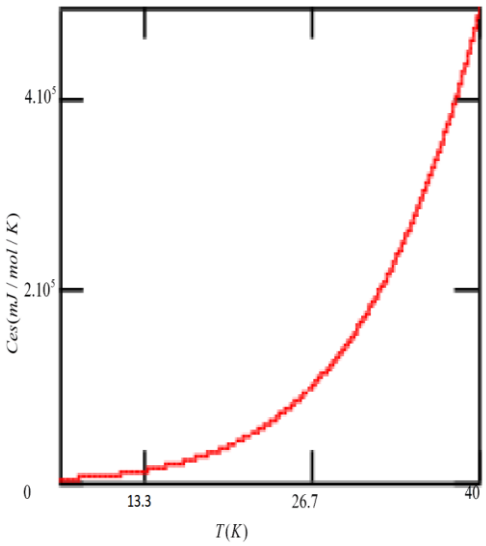

Fig 1: Variation of electronic specific heat in mJ/mol/K and temperature in Kelvin.

The variation of electronic specific heat C_{es} with temperature shows nonlinear increase in electronic specific heat with increase in temperature. In conformity with experimental data, is very low at low temperatures in the range of 0K-15K. Above 15K, the growth of C_{es} with temperature is exponential and asymptotic as it approaches 40K. We compare our result with Schriefer J.R (2013**)** shown in figure 2

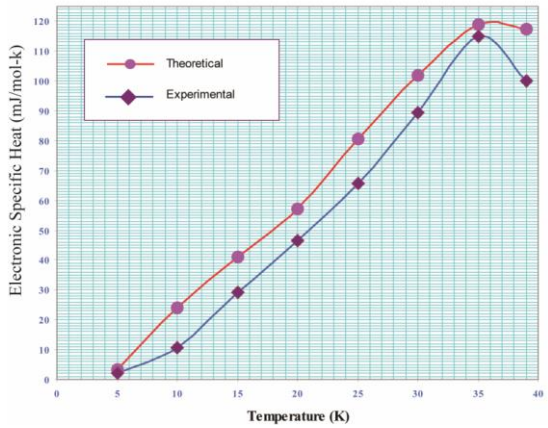

Figure 2: Variation of Electronic specific heat with temperature for both p and d bands adopted from Schriefer J.R (2013).

We also see nonlinear increase, C_{es} with temperature but optimized at 35K, where there is a sharp nonlinear fall in electronic specific heat.

2.9.2 Energy verses temperature

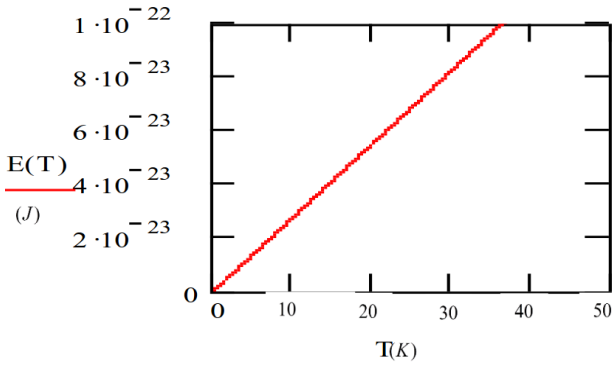

Figure 5.6. Variation of energy verses Temperature.

The trend is linear. The graph describes thermal energy between molecules within magnesium diboride system and is a measure of change and a property possessed by the system in a short time. While temperature describes the average kinetic energy of molecules within magnesium diboride system, and it is a measurable property of the system also known as a state variable.

The trend deviates slightly from that shown by Cuprates (Rapando et. al 2015). Which shows low growth rate of energy in the temperature range of 0K-100K but a high growth rate between 100K and 300K. Beyond 300K the cuprates exhibit very reduced increase in energy with temperature. The difference could be as a result of the 'abnormal' behavior of MgB_2. Its behavior at transition is more of a metallic superconductor than a cuprate. While in Cuprates, energy is drastically reduced at transition because of phonon-mediated pairing with both both electrons in the Cooper pair having similar properties, in the MgB_2 the two electrons that pair have different properties. The electron in the sigma bonding is found to be strongly superconducting while the one in the Pi bonding is less superconducting- more of normal electron. This gives MgB_2 more metallic properties.

Conclusions.

In the search for a suitable method of explaining microscopic mechanisms that allow superconductivity to occur at high temperature, we have shown superconducting in MgB_2 by canonical two band BCS Hamiltonian containing Fermi surfaces of p and d bands. The envisaged interaction of phonon mediated attraction and coulomb repulsion was proposed to act differently on energy band states and stabilizing superconductor phase for MgB_2 to unearth the mystery of microscopic mechanisms that allow superconductivity to persist at such high temperatures.

Following Bogoliubov -Valatin technique method, we obtained expressions for electron-phonon interaction model Hamiltonian for two band model isotope, expression for variation of thermodynamic properties with temperature and, which were the objectives of the study. Using the values of various parameters for a system MgB_2, we have made study of various physical properties and wherever possible, compared our results with available experimental data.

1. The statistical thermodynamics of high T_C superconductors in two band model considered interaction of phonon mediated attraction and coulomb repulsion and achieved its objectives by formulating an effective Hamiltonian diagonalized by B.V,T, energy of the MgB_2 system, specific heat capacity equation and its value.

2. The temperature dependent on two superconducting gaps Δ_p and Δ_d corresponding to p and d bands for MgB_2 was found. The two gaps structure is perfectly in agreement with experimental observations and values.

3. The specific heat behavior obtained from our model verses Temperature is in satisfactory agreement with experimental results, although the theoretical values are slightly higher than the experimental values which are attributed to mean field approximations.

4. The density of states behavior is similar to BCS weak coupling superconductors. This reveals that MgB_2 superconductors resembles to that of high T_C cuprates but the density of states for the system MgB_2 is quite high.

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