Theoretical Study of Density of States of Magnesium Diboride Superconductor based on Multi Band Model

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Abstract— Magnesium diboride with Tc = 39K is a record breaking compound among s-p metals & alloys. Many experiments performed on Magnesium diboride suggest that there are two superconducting gaps. Considering a multiband model Hamiltonian with intra- & inter band pair transfer interactions we have derived the normal and anomalous one-particle Green's function & self-consistent equations for superconducting order parameter(Δ) using Green's function technique & equation of motion method, we have studied the density of states. The results are quite encouraging.

Key words: Two band superconductivity, Hamiltonian, Green's functions, Superconducting order parameter, Density of states

I. INTRODUCTION

Magneisum diboride is an old material, known since early 1950's but it was discovered to be a superconductor by Nagamatsu et al.[1]at a remarkably high temperature about 39K. This discovery certainly received the interest of many researchers in the field of superconductivity especially in non oxides & initiated a search for superconductivity in related boron compounds [2]. Magnesium diboride is receiving attention due to exceptionally high values of critical temperature & critical field. This material may be suitable contender to replace Nb3Sn or NbTi as the choice for practical large scale application in the range of 20-30K operating with cryogenic refrigerators.

MgB2 possesses the simple hexagonal AlB2 type structure. It contains graphite type boron layers which are separated by closed packed layers of magnesium. Magnesium atoms are located at the centre of hexagons formed by borons. Band structure calculation of MgB2 reveals that there are two types of bands with two superconducting gaps in the excitation spectrum at the Fermi surface. The first one is a heavy hole band built up of σ band orbital & the second one is the broader band built up mainly of π band orbital [3-7]. It is a established fact that MgB2 is an anisotropic two gap superconductor [4]. Both the energy gaps have s-wave symmetries; the larger gap is highly anisotropic while the smaller one is slightly anisotropic. It is natural to describe a two gap superconductor by means of a two band model with inter band coupling [8-9]. There is a number of two band type approaches for superconductivity in magnesium diboride [10]. Two band models have been exploited in various realisations for cuprate superconductivity. Liu et al. [4] pointed the role of electron-phonon interaction between σ & π bands in magnesium diboride. Using two band models, we studied the superconducting order parameter & density of states of magnesium diboride.

II. MODEL HAMILTONIAN:

We start with two bands Hamiltonian with intra & inter band pair transfer interactions [11].

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

Where $\bar{\in}_{\alpha}=\in_{\alpha}-\mu$ is the electron energy in the bands α =1, 2; μ is the chemical potential; V is the volume of the superconductor & $W_{\alpha\alpha'}(l,m)$ are the matrix elements of intraband or interband interactions, if $\alpha=\alpha'$ or $\alpha\neq\alpha'$, respectively.

Using above Hamiltonian, we obtained following Green function

$$G_{11}=-\frac{\left[(\omega+\tilde{\in}_1)\{(\omega^2-\tilde{\in}_2^2)-W'^2-(\omega+\tilde{\in}_2)W_{12}\gamma\}-(\omega-\tilde{\in}_2)W_{12}^2\gamma^2\right]}{2\pi\left[(\omega^2-\tilde{\in}_1^2)(\omega^2-\tilde{\in}_2^2)-(\omega^2-\tilde{\in}_1^2)W'^2-(\omega^2-\tilde{\in}_2^2)W^2-2W_{12}^2\gamma^2(\omega^2+\tilde{\in}_1\tilde{\in}_2)\right]} \quad (2)$$

Where

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

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

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

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

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

$$\Delta_{11}=\frac{1}{V}\left\langle a_{1-k\downarrow}a_{1k\uparrow}\right\rangle \qquad \Delta_{22}=\frac{1}{V}\left\langle a_{2-k\downarrow}a_{2k\uparrow}\right\rangle$$

$$\Delta^{+}_{11}=\frac{1}{V}\left\langle a^{+}_{1k\uparrow}a^{+}_{1-k\downarrow}\right\rangle \qquad \Delta^{+}_{22}=\frac{1}{V}\left\langle a^{+}_{2k\uparrow}a^{+}_{2-k\downarrow}\right\rangle$$

$$W=W_{11}\Delta_1+W_{12}\Delta_2 \qquad W'=W_{12}\Delta_1+W_{11}\Delta_2$$

In obtaining Green's functions, we have assumed

$$W_{12}=W_{21}, \quad W_{11}=W_{22}, \quad \gamma_{12}=\gamma_{21}=\gamma$$

$$\frac{N_s(\omega)}{N(0)}=\frac{W_{12}\gamma}{\pi(\omega^2-W_{12}^2\Delta_2^2)}\left[-\frac{\omega^2}{\sqrt{\omega^2-W_{11}^2\Delta_1^2}}+W_{12}\gamma\right]$$

$\Delta_{11}=\Delta^{+}_{11}=\Delta_1$ & $\Delta_{22}=\Delta^{+}_{22}=\Delta_2$

On further simplification, one obtain

$$G_{11}=\frac{1}{4\pi\alpha_1\alpha_2^2(\alpha_1^2-\alpha_2^2)}\left[\frac{X+Y}{(\omega-\alpha_1)}+\frac{X-Y}{(\omega+\alpha_1)}\right]+\frac{W_{12}\gamma}{4\pi\alpha_2(\alpha_1^2-\alpha_2^2)}\left[\frac{X_1+Y_1}{(\omega-\alpha_2)}+\frac{X_1-Y_1}{(\omega+\alpha_2)}\right] \quad (3)$$

Where

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

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

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

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

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

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

We obtain the correlation function for the Green's function given by equation (3) as,

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

III. PHYSICAL PROPERTIES:

A. Superconducting order parameter:

Using above correlation function, we have obtained Superconducting order parameter (Δ) given by

$$\Delta=2N(0)|g|\int_0^{\hbar\omega_D}\left[\begin{array}{l}\dfrac{W}{4\pi\left(\alpha_1^2-\alpha_2^2\right)}\left\{\alpha_1\tanh\left(\dfrac{\beta\alpha_1}{2}\right)-\alpha_2\tanh\left(\dfrac{\beta\alpha_2}{2}\right)\right\}\\ -\dfrac{\left\{W\,\tilde{\in}_2^{\,2}+W_{12}\gamma\left(W\,\tilde{\in}_2+W'\,\tilde{\in}_1\right)\right\}}{4\pi\left(\alpha_1^2-\alpha_2^2\right)}\left\{\dfrac{1}{\alpha_1}\tanh\left(\dfrac{\beta\alpha_1}{2}\right)-\dfrac{1}{\alpha_2}\tanh\left(\dfrac{\beta\alpha_2}{2}\right)\right\}\end{array}\right]d\in_\alpha \quad (5)$$

Where W, W $^{/}$, α_1 and α_2 are defined in previous section and

$$\tilde{\in}_1=\in_1-\mu-\frac{W_{11}}{2}\quad\text{And}\quad\tilde{\in}_2=\in_2-\mu-\frac{W_{11}}{2}$$

B. Density of states:

For ω > 0, the density of states per atom N (ω) is defined as [12, 13]

$$N(\omega)=\lim_{\in\to 0}\frac{1}{2\pi}\sum_K\left[G_{11}(K,\omega+i\in)-G_{11}(K,\omega-i\in)\right]$$

Using G_{11} from eq. (3), we get

$$\frac{N_1(\omega)}{N(0)}=\frac{1}{\pi}\left[\frac{\omega}{\sqrt{\omega^2-W_{11}^2\Delta_1^2}}-W_{12}\gamma\frac{\omega}{\omega^2-W_{11}^2\Delta_1^2}\right] \quad (6)$$

&

$$\frac{N_2(\omega)}{N(0)}=\frac{W_{12}\gamma}{\pi\left(\omega^2-W_{12}^2\Delta_2^2\right)}\left[-\frac{\omega^2}{\sqrt{\omega^2-W_{11}^2\Delta_1^2}}+W_{12}\gamma\right] \quad (7)$$

IV. NUMERICAL CALCULATIONS:

We now evaluate numerically density of states using following parameters given in Table 1 for MgB_2.Choosing
W_{11}= W_{22}=0.3 eV.cell = 9.6x 10^{-21}J γ = (-) 0.01753
W_{12}= W_{21}= z eV.cell = z x 32x10^{-21}J Δ_1 = x for z = 0.0001

$$\frac{N_1(\omega)}{N(0)}=0.31847\left[\frac{y}{\sqrt{y^2-92.16x^2}}+\frac{0.0000561y}{y^2-92.16x^2}\right] \quad (8)$$

&

$$\frac{N_2(\omega)}{N(0)}=\frac{0.00001787}{\left(y^2-0.00001024x^2\right)}\left[\frac{y^2}{\sqrt{y^2-92.16x^2}}-0.0000561\right] \quad (9)$$

V. DISCUSSIONS & CONCLUSIONS:

In the previous sections, we have presented the study of superconductivity in magnesium diboride based on multiband Hamiltonian with intra & inter band pair transfer interactions. Following the Green's function technique & equation of motion method, we have obtained the expressions for superconducting order parameters Δ_1, Δ_2 and $\Delta = \Delta_1 + \Delta_2$ as well as for density of states. Making use of various parameters given in Table 1 for the system MgB_2, we have studied the above cited physical properties.

The variation of density of states N (ω)/N (0) with ω for value of matrix element of inter band interaction W_{12}= 0.0001 eV.cell have been studied at different temperatures & is shown in figure 1 & 2. The dashed curve is obtained from the BCS theory. The results obtained are quite encouraging & just similar to type I superconductors. It is clear from the figure that the level moves below the band due to interband & intraband interactions.

Two band mechanisms emerge as a strong contender for an acceptable model for MgB2 – inter metallic binary compounds. The efforts to understand the pairing mechanism in MgB2 & other similar systems should be continued, for such efforts go hand –in-hand with enhancing future prospectus for new superconducting materials & novel applications [14-21].

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S. No.	Parameter	Value	Reference
1	Pairing Interaction $W_{11}=W_{22}$ intraband	0.3 eV.cell	[11]
2	Pairing Interaction $W_{12}=W_{21}$ interband	0.0001eV.cell	[11]

Table 1: Values of various parameters for Magnesium Diboride (MgB2) system

S. No.	Frequency $\omega = y X 10^{-21}$	Density of states			
		BCS	10K	20K	30K
1	6	0.32062	0.32261	0.32222	0.32080
2	6.5	0.32029	0.32198	0.32165	0.32045
3	7	0.31998	0.32149	0.32121	0.32018
4	7.5	0.31980	0.32110	0.32085	0.31995
5	8	0.31965	0.32078	0.32056	0.31977
6	8.5	0.31951	0.32051	0.32032	0.31962
7	9	0.31942	0.32029	0.32012	0.31950
8	9.5	0.31931	0.32010	0.31995	0.31939
9	10	0.31923	0.31994	0.31980	0.31930
10	10.5	0.31915	0.31981	0.31968	0.31922
11	11	0.31911	0.31968	0.31957	0.31916
12	11.5	0.31905	0.31958	0.31947	0.31910
13	12	0.31901	0.31949	0.31939	0.31904
14	12.5	0.31897	0.31941	0.31932	0.31900
15	13	0.31892	0.31934	0.31925	0.31896
16	13.5	0.31888	0.31927	0.31920	0.31892
17	14	0.31885	0.31922	0.31914	0.31889
18	14.5	0.31883	0.31917	0.31910	0.31886
19	15	0.31881	0.31912	0.31906	0.31884

Table 2: Density Of States {N1(Ω)/N(0)} At Different Temperatures For Magnesium Diboride (Mgb2) System

S. No.	Frequency $\omega = y X 10^{-21}$	Density of states		
		T=10K	T=20K	T=30K
1	9	8.787E-06	2.2679E-06	2.0184E-06
2	9.5	4.8827E-06	2.1158E-06	1.9089E-06
3	10	3.7145E-06	1.9845E-06	1.8108E-06
4	10.5	3.0923E-06	1.8698E-06	1.7224E-06
5	11	2.6896E-06	1.7686E-06	1.6423E-06
6	11.5	2.4010E-06	1.6786E-06	1.5695E-06
7	12	2.1808E-06	1.5798E-06	1.5028E-06
8	12.5	2.0055E-06	1.5248E-06	1.4417E-06
9	13	1.8616E-06	1.4586E-06	1.3853E-06

10	13.5	1.7407E-06	1.3982E-06	1.3333E-06
11	14	1.6371E-06	1.3428E-06	1.2850E-06
12	14.5	1.5472E-06	1.2918E-06	1.2401E-06
13	15	1.4682E-06	1.2448E-06	1.1983E-06

Table 3: Density of States {N2(Ω)/N(0)} At Different Temperatures For Magnesium Diboride (Mgb2) System

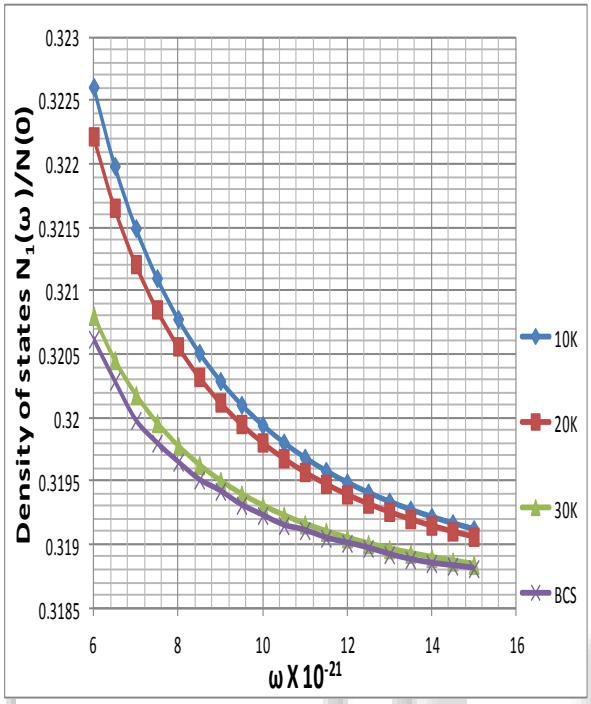

Fig. 1 Density of states 1 at different temperature for MgB_2

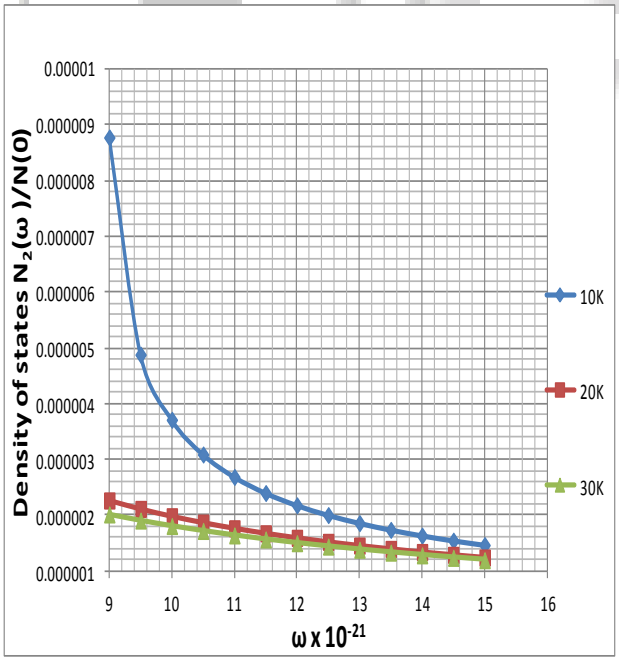

Fig. 2 Density of states 2 at different temperature for MgB_2