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IMPACT OF EXCHANGE-CORRELATION FUNCTIONS ON THE SUPERCONDUCTING PARAMETERS OF BINARY ALLOY MgB_2

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ABSTRACT

Magnesium Diboride has attracted the attention of physicists all over the world due to its characteristics band structure and high superconducting(SC) transition temperature 39K. In the present paper the superconducting(SC) state parameters λ, μ* and Tc representing the electron-phonon coupling strength, Coulomb - coupling strength and SC transition temperature of MgB_2 have been studied through Harrisons First Principle Pseudopotential [HFPP] technique[1]. The non-local screen form factor w(**k**, **q**) of the constituents have been computed through for widely excepted forms of exchange-correlation functions viz. Vashishta Singwi (V-S), Hubbard Sham (H-S), Kleimn -Langreth(K-L) and Shaw (SH) forms. The form factor of MgB_2 has been obtained through the well-known Faber-Ziman [2]. The SC state parameters have been completed through the Mc Millan's Formalism [3]. Reasonable agreement has been obtained with previous and experimental data.

KEY WORDS : Pseudopotential, Superconducting Parameters and Magnesium Diboride(MgB_2)

1. INTRODUCTION :

In the present era superconductivity(SC) occupies the centre stage due to its application on advanced technologies. Experimental work is being done at national and international level on superconductors. The theoretical investigations in this field are found to be lage behind the experiment in generating a suitable theory for the investigation of superconducting parameters of superconductors.

Magnesium diboride(MgB_2) is a simple superconducting material with layer structure. The boron atoms forms hexagonal honey combed planes and the planes of magnesium are located at the centre of hexagonal in between the boron planes. This system does not contain any transition metal.

The superconducting behavior of magnesium diboride(MgB_2) with high transition temperature (Tc = 39K) has sparked renewed interest in the system [4]. The high Tc appearance in such a simple system has lead to quite encouraging among the workers achieving the high value of Tc from the theoretical and experimental point of view.

The phonon mediated BCS theory is a good tool for the theoretical study of such a binay alloys using Mc Millan's formalism [3] in which Harrison's First Principle Pseudopotential [HFPP] technique [1] is used. Later Allen and Cohen [5] and their co-workers have used the BCS theory to explain the superconducting behavior of (MgB_2) [6]. The theory was extended to binary alloys by Allen and Dynes [7]. Recently scattered atoms have been made to apply Harrison' First Principle Pseudopotential [HFPP] technique [1] and we have also pursued our investigation along these lines.

2. FORMALISM :

The Harrison's First Principle Pseudopotential [HFPP] form factor of the metal is given by

$$w(\boldsymbol{k},\boldsymbol{q}) = \left[\frac{V_q^{a,b}+V_q^c+V_q^d}{\epsilon^*(q)}\right] + \left[\frac{\{1-G(q)\}}{\epsilon^*(q)}V_q^f + W_R\right] \quad \text{----------(1)}$$

where **k**, **q** are the electronic wave vector and phonon wave vector, $V_q^{a,b}$, V_q^c, V_q^d and V_q^f are the valance charge and core-electron potential, the conduction band-core exchange potential, the conduction electron potential and the screening potential. W_R is the repulsive potential, G(q) is the exchange-core relation function and $\epsilon*$(q) is the modified Hartree dielectric screening function.

The modified dielectric screening function $\in^*(q)$ is given by

$$\in^*(q) = (1-G(q))(\in(q)-1)+1 \quad \text{----------(2)}$$

ϵ(q) = Hartree dielectric screening function

$$= 1 + \frac{2}{\pi k_F \eta^2}\left[1 + \frac{4-\eta^2}{4\eta} ln\left|\frac{2+\eta}{2-\eta}\right|\right] \quad \text{----------(3)}$$

where $\eta = q/k_F$

Various forms of exchange-correlation functions are the following

Hubbard-Sham(H-S) function

$$G(q) = \frac{1}{2}\frac{\eta^2}{\eta^2+\beta+1} \quad \text{----------(4)}$$

where $\beta = k_s^2/k_F^2$ and $k_s = (4k_F/\pi)^{1/2}$

Kleinmann – Langreth (K-L) form

$$G(q) = \frac{1}{4}\frac{\eta^2}{\eta^2+\beta+1} + \frac{\eta^2}{\beta+1} \quad \text{----------(5)}$$

Shaw (SH) form :

$$G(q) = 1 - \exp(-0.535\eta^2) \quad \text{----------(6)}$$

Vashista-Singwi(V-S) form :

$$G(q) = A(1 - e^{B\eta^2}) \quad \text{----------(7)}$$

where A and B are V-S constants.

The V-S form is superior to other forms as it satisfied the compressibility some rule almost exactly and also provides better result of correlation function which is physically acceptable

The non-local screen form factor of the alloy using Faber-Ziman formalism is given by $|w(\boldsymbol{k},\boldsymbol{q})_{\boldsymbol{12}}|^2 = c_1|w(\boldsymbol{k},\boldsymbol{q})_{\boldsymbol{1}}|^2 + c_2|w(\boldsymbol{k},\boldsymbol{q})_{\boldsymbol{2}}|^2 + 2(c_1c_2)^{1/2}|w(\boldsymbol{k},\boldsymbol{q})_{\boldsymbol{1}}||w(\boldsymbol{k},\boldsymbol{q})_{\boldsymbol{2}}|$ -(8)

where $w(\mathbf{k},\mathbf{q})_1$ and $w(\mathbf{k},\mathbf{q})_2$ are the form factors of Mg and B respectively and $w(\boldsymbol{k},\boldsymbol{q})_{\boldsymbol{12}}$ is the form factor of MgB_2. c_1 and c_2 are the concentration fractions of Mg and B respectively.

The SC parameters under investigations have been computed through Mc Millan's formalism [3].

The electron-phonon coupling strength is given by

$$\lambda = \frac{12m^*z^*}{M<\omega^2>}\int_0^{2k_F} q^3|w(\boldsymbol{k},\boldsymbol{q})|^2 dq \quad \text{----------(9)}$$

where m^*, $z^*$and M are the effective mass of the electron, effective valance of the electron and atomic mass of the electron. $<\omega^2> = (k_B\Theta_D)^2$ is the averaged phonon frequency.

The Coulomb Pseudopotential is given by

$$\mu^* = \frac{\frac{m_b}{\pi k_F}\int_0^{2k_F}\frac{dq}{q[\epsilon^*(q)]}}{\left[1+\left(\frac{m_b}{\pi k_F}\right)ln\left(\frac{E_F}{k_B\Theta_D}\right)\int_0^{2k_F}\frac{dq}{q[\epsilon^*(q)e]}\right]} \quad \text{------- ----------(10)}$$

Where m_b, E_F, k_B and Θ_D are the band masss of the electron, the Fermi energy of the alloy, the Fermi wave vector of the alloy, the Boltzmann's constant of the alloy and Debye temperature respectively.

The SC transition temperature is given by

$$T_C = \frac{\Theta_D}{1.45} exp\left[-\left(\frac{1.04(1+\lambda)}{\lambda-\mu^*(1+0.62\lambda)}\right)\right] \quad \text{----------(12)}$$

The Debye temperature of the alloy is given by

$$\frac{1}{(\Theta_D)_{12}^2} = \frac{1-c_1}{(\Theta_D)_1^2} + \frac{c_2}{(\Theta_D)_2^2} \quad \text{----------(13)}$$

3. COMPUTATION:

In this section we study the impact of four popular type of exchange-correlation function [G(q)] namely- Vashishta-Singwi(V-S), Hubbard-Sham(H-S), Kleinman-Langreth(K-L) and Shaw(SH) forms on the computation of non-local screened form factors of the constituents. The form factors of the constituents using different forms of exchange-correlation functions have been used for the computation of the above SC state parameters of MgB_2.The computation of the form factors w(**k**,**q**) has been done by using equation (1) and the modified hartree dielectric screening function ϵ^* is carried on through equations (2) and (3) for the computation of w(**k**,**q**), the core energy eigenvalues (ϵ_{nl}) is taken from Herman-Skillman (H-S) [12] and Clementi (C) [13]. From the computed form factors $w(\mathbf{k},\mathbf{q})_1$ and $w(\mathbf{k},\mathbf{q})_2$ of the metals Mg and B, the form factor $w(\mathbf{k},\mathbf{q})_{12}$ of the binary alloy MgB_2 is obtained through equation(8) and the Debye temperature of alloy is obtained through equation (13). The computed form factors of MgB_2 for the two sets of core - energy eigenvalues Herman-Skillman(H) and Clementi(C) using Xα-exchange parameter ($\alpha=2/3$) and orthogonalization hole parameter ($\beta=5/8$) at different exchange-correlation functions have been presented in Table 1 and Table 2. After these computations we proceed to compute the superconducting parameters through equations (9),(10) and (11). The nature of computed form factors have been shown in Fig1 and Fig2 for comparison. The results of the computed SC parameters have been presented in Table 3 alongwith the theoretical data of the other previous authors as well as the experimental data.

4. RESULTS AND DISCSSION:

From Table (1) and (2) it is found that the form factors of MgB_2 using H and C eiginvalues with $\alpha=2/3$ and $\beta=5/8$ computed through Vashishta-Singwi(V-S), Hubbard-Sham(H-S) and Kleinman-Langreth(K-L) form of exchange-correlation functions lie in the vicinity of each other throughout the entire range of η.

Table 1

Form factors of MgB_2 (in Ryd.) using H eigenvalues with $\alpha=2/3$ and $\beta=5/8$ at different exchange-correlation functions

$\eta = q/k_F$	$w(\mathbf{k},\mathbf{q})_{V\text{-}S}$	$w(\mathbf{k},\mathbf{q})_{H\text{-}S}$	$w(\mathbf{k},\mathbf{q})_{K\text{-}L}$	$w(\mathbf{k},\mathbf{q})_{SHAW}$
0.0	-1.0089	-1.0089	-1.0089	-1.0089
0.2	-1.0353	-1.0343	-1.0333	-1.0454
0.4	-0.9736	-0.9693	-0.9668	-1.0072
0.6	-0.8660	-0.8557	-0.8541	-0.9203
0.8	-0.7320	-0.7164	-0.7181	-0.7921
1.0	-0.5906	-0.5739	-0.5786	-0.6398
1.2	-0.4563	-0.4437	-0.4493	-0.4858
1.4	-0.3385	-0.3332	-0.3369	-0.3491
1.6	-0.2413	-0.2438	-0.2438	-0.2395
1.8	-0.1652	-0.1732	-0.1692	-0.1581
2.0	-0.1048	-0.1119	-0.1073	-0.0998

Table 2

Form factors of MgB_2 (in Ryd.) using C eigenvalues with $\alpha=2/3$ and $\beta=5/8$ at different exchange-correlation functions

$\eta = q/k_F$	$w(\mathbf{k},\mathbf{q})_{V\text{-}S}$	$w(\mathbf{k},\mathbf{q})_{H\text{-}S}$	$w(\mathbf{k},\mathbf{q})_{K\text{-}L}$	$w(\mathbf{k},\mathbf{q})_{SHAW}$
0.0	-1.0089	-1.0089	-1.0089	-1.0089
0.2	-1.0365	-1.0355	-1.0345	-1.0466
0.4	-0.9749	-0.9705	-0.9680	-1.0085
0.6	-0.8672	-0.8568	-0.8551	-0.9217
0.8	-0.7338	-0.7178	-0.7190	-0.7945
1.0	-0.5937	-0.5759	-0.5800	-0.6445
1.2	-0.4615	-0.4467	-0.4517	-0.4938
1.4	-0.3461	-0.3374	-0.3409	-0.3604
1.6	-0.2514	-0.2493	-0.2496	-0.2534
1.8	-0.1776	-0.1802	-0.1773	-0.1737
2.0	-0.1195	-0.1223	-0.1191	-0.1164

Table 3

Computed SC state parameters using $\alpha=2/3$ and $\beta=5/8$ alongwith H and C eigenvalues for different exchange-correlation functions

Form factors	**SC State Parameters**						
	μ*	**λ (Present)**		**λ (Previous)**	**T_C(Present)(K)**		**T_C (Exp.)(K)**
		H	C		H	C	
$w(\mathbf{k},\mathbf{q})_{V\text{-}S}$	0.11	0.79	0.82	~ 0.7-0.9[1-5]	36.4	39.9	39K[6-7]
$w(\mathbf{k},\mathbf{q})_{H\text{-}S}$	0.11	0.77	0.79	-	34.9	37.0	-
$w(\mathbf{k},\mathbf{q})_{K\text{-}L}$	0.11	0.78	0.80	-	35.3	37.4	-
$w(\mathbf{k},\mathbf{q})_{SH}$	0.11	0.86	0.91	-	43.7	48.3	-

[1] Kortous et. Al (2001)
[2] An J M et. Al (2001)
[3] Kong et. al (2001)
[4] Liu et. al (2001)
[5] Yildrim et. al (2001)
[6] Akimitsu (2001)
[7] Nagamatsu et. al (2001)

η

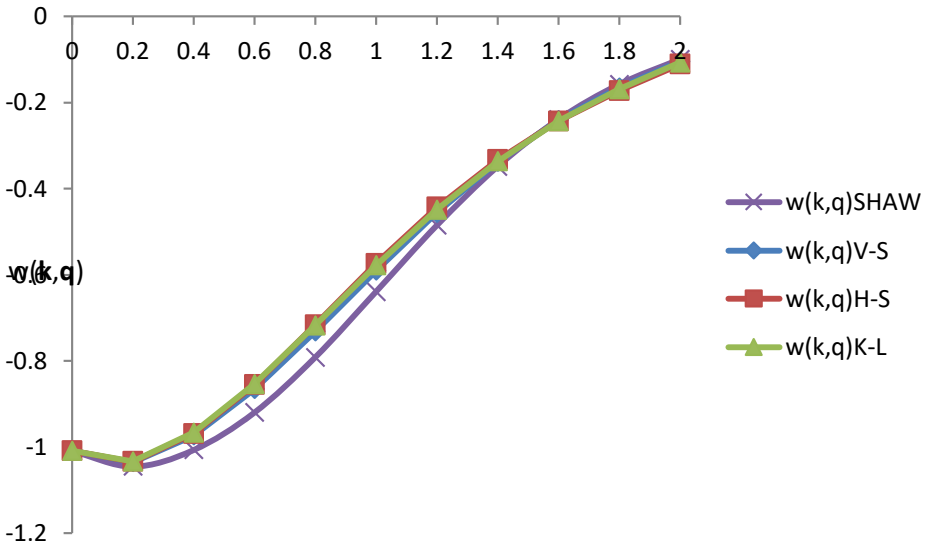

Fig1. Computed form factor w(k,q) of MgB_2 (in Ryd.) using H eigenvalues with α =2/3 and β = 5/8 at different exchange-correlation functions

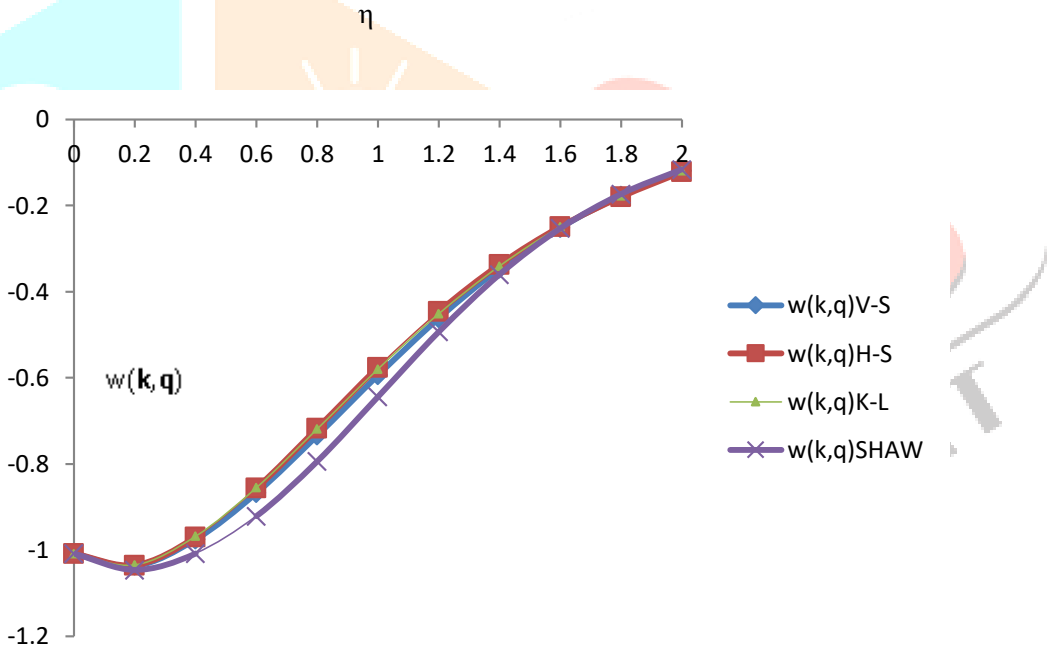

Fig2. Computed form factor w(k,q) of MgB_2 (in Ryd.) using C eigenvalues with α =2/3 and β = 5/8 at different exchange-correlation functions

The form factor computed though Shaw(SH) form of exchange- correlation function shows larger variation in magnitude up to η < 1.6 than the form factors obtained by other and the small variation in magnitude beyond η > 1.6 than obtained by other. The form factors computed through Hubbard-Sham(H-S) and Kleinman-Langreth(K-L) are smallest variation up to η<1.6 and largest variation in magnitude beyond η>1.6. The form factor compted through Vashishta-Singwi(V-S) form lies in between these two. At η = 2.0 all the form factors nearly converge.

Table 3 reveals that the Coulomb Pseudopotential strength μ* is found to be of the order of 0.1 as obtained by the previous authors. The value of electron-phonon coupling strength λ with α=2/3 and β=5/8 lies in the range of 0.79 - 0.82, 0.77-0.79, 0.78-0.80 and 0.86-0.91. However λ lies in the range of 0.7-0.9 as obtained by previous authors. The value of transition temperature T_C lies in the range of 36.4-39.9, 34.9-37.0, 35.3-37.4 and 43.7-48.3 against the experimental value of T_C=39K. The impact of λ is about 0.03 [λ_H = 0.79,λ_C = 0.82], 0.02 [λ_H = 0.77,λ_C = 0.79], 0.02 [λ_H = 0.78,λ_C = 0.80] and 0.05 [λ_H = 0.86,λ_C = 0.91]. The impact of T_C is about 3.5 [T_C(H) =36.4K, T_C(C) =39.9K], 2.1 [T_C(H)

=35.3K, T_C(C) =37.4K] and 4.6 [T_C(H) =43.7K, T_C(C) =48.3K]. Thus C eigenvalue obtained by (V-S) form of exchange-correlation function with $\alpha=2/3$ and $\beta=5/8$ give better agreement 39.9K against the experimental T_C =39K

4. CONCLUSION:

HFP Psedopotential technique based on BCS theory and Mc Millan's formalism has been used to compute the electron-phonon coupling strength λ, Coulomb Psedopotential μ* and SC state transition temperature T_C of MgB_2. Using different exchange-correlation function the values of λ, μ* and T_C have been computed for the alloys of MgB_2. It has been seen that with Shaw form of exchange-correlation function both λ, and T_C are higher as the form factor is largest in respect of magnitude than the others. Our results are quite satisfactory as compared to the values obtained by previous researchers. Our computations reveals that SC parameters are reasonable reproducible by HFP Psedopotential Technique.

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