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## Pseudopotential study of the superconducting behaviour of $MgB_2$ : HFP technique

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### ABSTRACT

The study of recent literature reveals that the discovery of high  $T_c$  ( $T_c = 39K$ ) superconductivity (SC) in  $MgB_2$  has generated considerable interest in this binary system. The appearance of high  $T_c$  SC in such a simple system which does not contain transition metals has led to considerable optimism among workers. The phonon mediated BCS type mechanism has been acknowledged to be a good tool for its theoretical study via McMillan formalism. Recent studies are the milestones in this direction. In this paper, we report the Harrison's First Principle Pseudopotential (HFPP) study of this system so as to bring out the effectiveness of this technique which has not been explored as yet. It has been observed that due to the unique double layered structure of  $MgB_2$  some adjustable parameter is to be introduced in the computation of the form factor so as to predict the SC parameters in reasonable agreement with experiment.

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### KEYWORDS

Pseudopotential;  
Superconducting parameters;  
Magnesium diboride ( $MgB_2$ ).

### INTRODUCTION

Superconductivity is a property of many metals, alloys and chemical compounds at temperatures near absolute zero by virtue of which their electrical resistivity vanishes and they become strongly diamagnetic. The discovery of superconductivity (SC) in magnesium diboride ( $MgB_2$ ) with remarkable high transition temperature ( $T_c = 39K$ ) has generated considerable interest in this system<sup>[1]</sup>.  $MgB_2$  adopt a simple primitive hexagonal crystal structure comprising of interleaved two dimensional of magnesium and boron layers. The appearance of high  $T_c$  in such a simple system which does not contain transition metal is quite encouraging from

theoretical and experimental point of view. It has generated optimism for achieving high value of  $T_c$  in binary systems with simple constituents.

It has been noted that the theories developed to explain SC in the layered high  $T_c$  curates would not be helpful in understanding  $MgB_2$  and hence Loui and Cohen and their co-workers have used the well established BCS theory to explain the superconducting behaviour of  $MgB_2$ <sup>[2]</sup>. The phonon mediated BCS type of mechanism is a good tool for the study of such systems via McMillan formalism<sup>[3]</sup>. Recently such attempts are being made<sup>[4-7]</sup> and we have also persued over investigation along these lines using Harrison's first principle pseudopotential (HFPP) technique<sup>[8]</sup>.

## Formalism and computation

The HFPP form factor is represented as

$$w(\mathbf{k}, \mathbf{q}) = \left\{ \frac{v_q^{a,b} + v_q^c + v_q^d}{\epsilon^*(\mathbf{q})} \right\} + \left[ \frac{1 - G(\mathbf{q})}{\epsilon^*(\mathbf{q})} \right] v_q^f + W^R \quad (1)$$

where  $v_q^{a,b}$  is the valence charge and core electron potential,  $v_q^c$  is the conduction band-core exchange potential,  $v_q^d$  is the screening potential,  $W^R$  is the repulsive potential,  $\epsilon^*(\mathbf{q})$  is the modified Hartree dielectric screening function and  $G(\mathbf{q})$  is the exchange-correlation function. The potentials are computed from first principles on the lines of Harrison<sup>[8]</sup>.

The basic input parameters needed for the computation are the core energy eigenvalue  $\epsilon_{nl}$  radial wavefunctions  $P_{nl}(r)$ , Fermi wave vector  $k_F$ , atomic volume  $\Omega_0$  and valence  $Z$ . The pseudopotential form factor and other parameters of the binary system may be computed through

$$X_{AB} = (1-c)X_A + cX_B \quad (2)$$

where  $X_A$  and  $X_B$  are the parameters or the form factor of the constituents and  $X_{AB}$  those of the binary system,  $c$  is the concentration of the second constituent<sup>[9]</sup>.

The Debye temperature of the binary system is represented by<sup>[10]</sup>

$$1/(\theta_D)_{AB}^2 = (1-c)/(\theta_D)_A^2 + c/(\theta_D)_B^2 \quad (3)$$

The SC parameters have been computed through the McMillan formalism<sup>[3]</sup>. The electron-phonon coupling strength

$$\lambda = \frac{12m^*Z^*}{M \langle \omega^2 \rangle} \int_0^1 \eta^3 |w(\mathbf{k}, \mathbf{q})|^2 d\eta \quad (4)$$

where  $m^*$  is the effective mass of the electron,  $Z^*$  the effective valence,  $M$  the atomic mass,  $\langle \omega^2 \rangle$  the averaged phonon frequency and  $\eta = q/2k_F$ .

The Coulomb pseudopotential is represented by

$$\mu^* = [m_b/(\pi k_F)] I / [1 + m_b/(\pi k_F) \ln(E_F/k_B \theta_D) I] \quad (5)$$

$$\text{With } I = \int_0^1 d\eta / (\eta \epsilon^*(\eta)) \quad (6)$$

where  $m_b$  is the band mass,  $E_F$  the Fermi energy,  $k_B$  the Boltzmann's constant,  $\theta_D$  the Debye temperature and  $k_F$  the Fermi wave vector. The superconducting transition temperature is given by

$$T_c = \frac{\theta_D}{1.45} \exp \left[ \frac{-1.04(1+\lambda)}{\lambda - \mu^*(1+0.62\lambda)} \right] \quad (7)$$

The computation of the HFPP form factor has been done with Herman-Skillman<sup>[11]</sup> eigenvalues and eigenfunctions using  $X\alpha$  exchange parameters ( $\alpha_X$ ) satisfying Virial theorem and exchange-correlation function  $G(\mathbf{q})$  suggested by Vashishta-Singwi (V-S)<sup>[12]</sup> form which satisfies compressibility some rule and provides physically acceptable pair correlation function.

The results which are being presented are only those which reasonably agree with the experimental data of  $T_c$  and theoretical data of other authors. It was felt that  $MgB_2$  having special features as regards its structure mentioned earlier needs some adjustable parameter  $\beta$  in the form factor  $w(\mathbf{k}, \mathbf{q})$  so as to reproduce the reasonable agreement with experimental data  $T_c$ . For this Harrison prescription<sup>[8]</sup> has been adopted. Thus

$$w(\mathbf{k}, \mathbf{q}) = \langle \mathbf{k} + \mathbf{q} | w | \mathbf{k} \rangle \\ = (1+\beta) \langle \mathbf{k} + \mathbf{q} | w^0 | \mathbf{k} \rangle / \epsilon^*(\mathbf{q}) \quad (8)$$

with a suitable choice of  $\beta$  we can obtain a rather good form factor which can predict a reasonable value of  $T_c$ . The adjustable parameter  $\beta$  would throw light on the effect of double layered structure of  $MgB_2$ .

## RESULT AND DISCUSSION

It has been observed that the form factor of  $MgB_2$  is dominated by that of the boron atom. This implies the B-atoms in the boron layers play more.

It is known that at ambient conditions  $MgB_2$  crystallises in hexagonal structure where B-atoms form honeycomb lattice consisting of graphite like sheet separated by hexagonal layers of Mg atoms. The pairing mechanism leading to SC is of phononic origin. Thus the domination of B-atoms in shaping the form factor is quite natural. Gaitonde et al.<sup>[4]</sup> observes that the electronic band structure shows that the bands near the Fermi energy are predominantly due to the boron orbital. The flat bands contribute largely to the density of states near the Fermi level giving high  $T_c$ . In our computations also we observe that the most contributing part of the form factor  $w(\mathbf{k}, \mathbf{q})$  is in the region  $1 \leq \eta' \leq 2$  where  $\eta' = q/k_F$ . This is because the integrand involves the  $\eta^3$  and  $\Omega' |w(\mathbf{k}, \mathbf{q})|^2$  like Ziman integrand for electrical resistivity.

Two experimental values of the Debye temperature  $\theta_D = 750K$  and  $1050K$  are available<sup>[5]</sup> and employing these the original form factor  $w(\mathbf{k}, \mathbf{q})$  yields  $\lambda =$

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0.52,  $\mu^* = 0.09$ ,  $T_c = 9.95\text{K}$  and  $\lambda = 0.26$ ,  $\mu^* = 0.26$ ,  $T_c = 0.15\text{K}$ .

This shows that the ionic interactions are not properly reproduced as they exist in  $\text{MgB}_2$  structure and hence an adjustable parameter  $\beta$  has been introduced as

$$w(\mathbf{k}, \mathbf{q})_{AB} = (1 + \beta)[(1 - c)w(\mathbf{k}, \mathbf{q})_A + cw(\mathbf{k}, \mathbf{q})_B] \quad (9)$$

where  $c = 0.6666$  (stoichiometric composition).

With  $\theta_D = 750\text{K}$  and  $\beta = 0.3$  we get  $\lambda = 0.88$ ,  $\mu^* = 0.0944$ ,  $T_c = 36.8\text{K}$  and with  $\beta = 0.6$  we obtain  $\lambda = 0.83$ ,  $\mu^* = 0.0944$  and  $T_c = 37.2\text{K}$  ( $T_c = 39\text{K}$  expt.). With  $\theta_D = 1050\text{K}$  and  $\beta = 0.7$  we obtain  $\lambda = 0.77$ ,  $\mu^* = 0.0944$ ,  $T_c = 38.9\text{K}$ .  $\lambda$  has also been estimated by other techniques<sup>[4,5]</sup> with similar approximations and  $\lambda = 0.69$ ,  $\mu^* = 0.09$  and  $T_c = 30.8\text{K}$  has been obtained heat coefficient  $Y$  is given as

$$\lambda = Y_{\text{exp.}} / Y_{\text{calc.}} - 1 \quad (10)$$

$$\text{where } \lambda_{\text{calc.}} = 1/3\pi^2 D(E_F) k_B^2 \quad (11)$$

$D(E_F)$  being the density of states near Fermi level.  $Y_{\text{exp.}}$  has been reported to lie between 2.6-3 mJ/mol-K<sup>2</sup> which gives  $\lambda = 0.53$  and  $\lambda = 0.77$  respectively. Taking  $\mu^* = 0.1$ ,  $T_c = 9.4\text{K}$  and  $39\text{K}$  have been obtained with  $\theta_D = 750\text{K}$  and  $1050\text{K}$  respectively<sup>[5]</sup>. Thus our results with HFPP technique using  $\theta_D = 1050\text{K}$  agree with<sup>[5]</sup>. With  $\theta_D = 750\text{K}$  the result of<sup>[5]</sup> is  $T_c = 9.41\text{K}$  we have been able to improve the form factor by a 30% correction to accommodate the double layer interactions to get  $T_c = 36.8$  which is in reasonable agreement with experiment.

## CONCLUSION

The HFPP technique has been used to study the superconducting parameter of the high  $T_c$  superconductor  $\text{MgB}_2$  having double layered structure where boron atoms form honeycomb lattice separated by hexagonal layers of Mg atoms. The study reveals that an adjustable parameter should be introduced in the form factor  $w(\mathbf{k}, \mathbf{q})$  to take account of this special structure of  $\text{MgB}_2$  leading to superconducting behaviour with  $T_c = 39\text{K}$ . It has been observed that the form factor should be at least 30% more negative to consolidate the inter ionic interactions and reproduce the observed transition temperature. This shows that the repulsive component  $W^R$  involved in the expression of the form factor is

weakened by a substantial amount in the formation of  $\text{MgB}_2$  structure. This invites further investigation either for the improvement of the formalism or for using other sets of wave functions, exchange-correlation or the orthogonalization hole parameters as previously adopted by various authors in the past decades for pseudopotential calculations.

## REFERENCES

- [1] J.Nagamats, N.Nakagawa, Y.Zentaani, J.Akimitsu; Nature, 41063 (2001).
- [2] Research News, Paul Preurs, 510, 486-6249 (2002).
- [3] W.L.McMillan; Phys.Rev., 167, 313 (1968).
- [4] D.M.Gaitonde, P.Modak, R.S.Rao, B.K.Godwal; Bull.Mat.Sci., 26, 131 (2003).
- [5] P.P.Singh; Bull.Mat.Sci., 26, 131 (2003).
- [6] E.Eaito, Taknenobu, T.Ito, Y.Iwasa, K.Prassides, T.Arima; J.Phys.Condens.Matt., 13, 1267 (2001).
- [7] H.J.Choi, D.Roundy, H.Sun, M.L.Cohen, S.J.Louie; Letters to Nature, 418, 758 (2002).
- [8] W.A.Harrison; Pseudopotential in the Theory of Metals', Benjamin Inc.NY, (1966).
- [9] H.Khan, K.S.Sharma; UPAP, 36, 523 (1998)
- [10] S.Sharma, H.Khan, K.S.Sharma; UPAP, 41, 301 (2003).
- [11] F.Herman, J.Skillman; 'Atomic Structure Calculation', Prentice Hall Englewood Life, NJ.
- [12] P.Vashishta, K.S.Singwi; Phys.Rev.Lett., 86, 577 (2001).
- [13] K.P.Bohen et al.; Phys. Rev., B6, 875 (1972).
- [14] J.Kourtus et al.; Phys.Rev., B64, 20501 (2001).
- [15] J.Kourtus et al.; Phys.Rev.Lett., 86, 1877 (2001).
- [16] S.L.Budko et al.; Phys.Rev.Lett., 86, 1877 (2001).
- [17] F.Bouquet et al.; Phys.Rev.Lett., 82, 47001 (2001).