# Impact of Orthogonalization Hole Parameter: ab Initio Study

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**Abstract:** In this paper, we report the Pseudopotential technique study of this system which have not been explored extensively for binary alloys so as to bring out the effectiveness of this technique. We have studied the impact of orthogonalization hole parameter on the superconducting (SC) parameters of $MgB_2$. In general it has been observed that the choice of eigenvalues has much more impact on the form factor than that of α and β. But here the impact of orthogonalization hole parameter (β) is more than that of the choice of eigenvalues.

Keywords: Pseudopotential, superconducting parameters, Magnesium diboride ($MgB_2$)

## INTRODUCTION

The phenomenon of superconductivity is the thrust area of the theoretical and experimental research in the field of material science all over the world. Superconductors have found their way in advanced research and technology and hence enjoy the attention of physicists for the fabrication of a variety of superconductors and the study of their Superconducting (SC) parameters. The pseudopotential techniques have not been used so extensively for binary alloys. In the previous **articles**[3,4] the theoretical frame work for the computation of superconducting (SC) state parameters namely the Coulomb pseudopotential $\mu^*$, the electron-phonon coupling strength λ, the SC transition temperature $T_C$ has been presented alongwith the formalism of pseudopotential technique.

In this article we shall study the impact of the orthogonalization hole parameter (β) on the computed form factors and the SC state parameters. When the localized charge density at a given ion is summed over all the wave numbers in the Fermi sphere it gives the positive charge distribution known as orthogonalization hole. The orthogonallization hole potential is involved in the energy dependent component $v_q^f$ and $W^R$ of the form factor through the core shift $f_{nl}$.

Harrison (1966) while dealing with multiple opw description of the states giving rise to screening, has observed that when the localised charge density at a given ion is summed over all wave numbers in the Fermi sphere it gives the positive charge distribution known as orthogonalization hole. It contains *–(Z*–Z)* electrons, where *Z** is the effective valence and Z is the valence (Harrison pp. 271 1966). Originally he has taken the orthogonalization hole potential $v_{opw}$ (vide. Eq **1**) without any reduction (i.e. β=1).

$$v_{OPW} = \frac{-\Omega}{\pi} 2\sum\nolimits_{nl} v_{nl} \int_0^{k_F} k^2 \, < k \mid nlo >^2 \, dk \tag{1}$$

where

$$v_{nl} = 2(2l+1)\int P_{nl}^2(r)/\, r dr \tag{2}$$

In $\langle k \,|\, nlo \rangle$ the symbol zero means m=0 and $k_F$ is the Fermi wave vector.

However, he has made an improved estimate of vopw through equations 8.36-8.38 (Harrison 1966) and shown that the previous estimate is 8/5 times higher. Hence a reduction factor β=5/8 was suggested (pp. 275 Harrison

1966). Later some authors followed this suggestion in computation of various physical properties. (Day et al 1977, King et al 1970, 1971, Hafner 1977).

It is to be mentioned that the orthogonalization hole potential $v_{opw}$ is involved in the core shift which is used in the expressions of $W^R$ the repulsive potential (vide. Eq **3**) and consequently $W^R$ is involved in the inner integrand of the screening potential $v_q^f$ (vide. Eq **4**).

$$W^R = \left\langle \mathbf{k}+\mathbf{q} \middle| W^R \middle| \mathbf{k} \right\rangle \tag{3}$$

$$v_q^f = 4\Big/\left(k_F \eta^3\right)\int_{-1}^{+1}\frac{dz}{\eta+2z}\int_0^{2k_F} dp\left\langle \mathbf{k}+\mathbf{q} \middle| W^R \middle| \mathbf{k} \right\rangle \tag{4}$$

Thus the reduction of $v_{opw}$ influences the form factor *w(k,q)* through the energy dependent components $W^R$ and $v_q^f$ in an intricate manner. In this way it is different from the Xα - exchange parameter which directly reduces the conduction band core exchange potential $v_q^c$ and consequently the form factor w*(k,q)*.

## COMPUTATION AND RESULT

We have observed that the Clementi eigenvalues (C) alongwith $\alpha = \alpha_{vt}$ (which satisfies the Virial theorem) gives a better picture of the computed SC state parameters λ (electron-phonon coupling strength) and $T_C$ (the superconducting transition temperature) with V-S form of exchange-correlation function. Thus in the present chapter the computation of form factor has been made with β=1 and β=5/8 retaining the other parameters mentioned above. The computed form factors have been given in Table 1 and presented in Fig 1.

However, for the sake of generality this investigation has also been done with H eigenvalues alongwith the $\alpha=\alpha_{vt}$ and V-S exchange correlation. The results have been presented in Table 2 and shown in Fig 2. The computed SC state parameters using these two sets of eigenvalues with β=1 and β=5/8 have been presented in Table 3.

## OBSERVATIONS

An inspection of Tables 5.1 and 5.2 reveals that for both the eigenvalues $w(k,q)_{\beta=5/8} < w(k,q)_{\beta=1}$ except in the lower range of η (η < 0.4).Thus the reduction of the orthogonalization hole parameter reduces the form factors in respect of magnitude in the higher region of η (η > 0.4). This has also been projected in Fig 5.1 and 5.2. The variations are not uniform they lie within the region 0.0015-0.0322 for H eigenvalues and 0.002-0.0251 for C eigenvalues (in Ryd.). The maximum percentage variation is 14.5% (for H eigenvalues) and 15.2% (for C eigenvalues). It may be noted that the maximum percentage variations due to the choice of different sets of eigenvalues was nearly 12% and that due to the choice of Xα-exchange parameters was of the order of 4% (vide. chapter III, chapter IV).

In general it has been observed that the choice of eigenvalues has much more impact on the form factor than that of α and β. But here the impact of β is more than that of the choice of eigenvalues. The reason for this seems to be the fact that among the two sets of eigenvalues both positive and negative deviations have been observed. Hence this cancellation effect has reduced the impact of different choices of eigenvalues. The alloying of magnesium and boron may be the other cause of such variations. A perusal of Table 5.3 reveals that with both sets of eigenvalues the electron-phonon coupling strength λ lies in the range of the data of previous authors even with β=5/8 but the SC state transition temperature $T_C$ is above the experimental value. Thus it is concluded that the reduction in $v_{opw}$ does not yield satisfactory agreement of $T_C$. Hence the Clementi eigenvalues alongwith $\alpha=\alpha_{vt}$, β=1 and V-S exchange-correlation have provided the nearest agreement.

In the next chapter we shall study the impact of various forms of exchange-correlation functions on the form factors as well as the SC state parameters.

TABLE– 5.1: Selected form factors of $MgB_2$ (in Ryd.) using C eigenvalues with $\beta=1$ and $\beta=5/8$ keeping $\alpha=\alpha_{vt}$ and (V-S) exchange correlation function.

| $\eta = w(k,q)$ | $w(k,q)_{\beta=1}$ | $w(k,q)_{\beta=5/8}$ | $\Delta w = w(k,q)_{\beta=1} - w(k,q)_{\beta=5/8}$ |
|---|---|---|---|
| 0.0 | -1.0089 | -1.0089 | 0 |
| 0.2 | -1.0394 | -1.0374 | +0.0020 |
| 0.4 | -0.9779 | -0.9785 | -0.0006 |
| 0.6 | -0.8688 | -0.8743 | -0.0055 |
| 0.8 | -0.7329 | -0.7441 | -0.0112 |
| 1.0 | -0.5899 | -0.6064 | -0.0165 |
| 1.2 | -0.4546 | -0.4754 | -0.0208 |
| 1.4 | -0.3366 | -0.3601 | -0.0235 |
| 1.6 | -0.2400 | -0.2649 | -0.0249 |
| 1.8 | -0.1648 | -0.1899 | -0.0251 |
| 2.0 | -0.1059 | -0.1306 | -0.0247 |

TABLE–5.2: Selected form factors of $MgB_2$ (in Ryd.) using H eigenvalues with $\beta=1$ and $\beta=5/8$ keeping $\alpha = \alpha_{vt}$ and (V-S) exchange correlation function.

| $\eta = w(k,q)$ | $w(k,q)_{\beta=1}$ | $w(k,q)_{\beta=5/8}$ | $\Delta w = w(k,q)_{\beta=1} - w(k,q)_{\beta=5/8}$ |
|---|---|---|---|
| 0.0 | -1.0089 | -1.0089 | 0 |
| 0.2 | -1.0377 | -1.0362 | +0.0015 |
| 0.4 | -0.9746 | -0.9772 | -0.0026 |
| 0.6 | -0.8635 | -0.8730 | -0.0095 |
| 0.8 | -0.7250 | -0.7423 | -0.0173 |
| 1.0 | -0.5790 | -0.6032 | -0.0242 |
| 1.2 | -0.4409 | -0.4701 | -0.0292 |
| 1.4 | -0.3206 | -0.3524 | -0.0318 |
| 1.6 | -0.2225 | -0.2547 | -0.0322 |
| 1.8 | -0.1470 | -0.1775 | -0.0305 |
| 2.0 | -0.1018 | -0.1159 | -0.0141 |

TABLE – 5.3: Computed SC state parameters using $\beta = 1$ and $\beta = 5/8$ alongwith H and C eigenvalues.

| Form factor | SC state parameters | | | | | | |
|---|---|---|---|---|---|---|---|
| | $\mu^*$ | $\lambda$ (Present) | | $\lambda$ (Previous) | $T_C$ (Present) | | $T_C$(Exp.) |
| | | $\beta = 1$ | $\beta = 5/8$ | | $\beta = 1$ | $\beta = 5/8$ | |
| $w(k,q)_C$ | 0.11 | 0.79 | 0.88 | ~ 0.7 – 0.9[1] | 36.1 | 45.7 | 39K [2] |
| $w(k,q)_H$ | 0.11 | 0.73 | 0.84 | | 30.2 | 42.0 | |

In chapter V the impact of orthogonalization hole parameter $\beta$ has been studied in respect of the form factor and also $\lambda$ and $T_C$. When the localized charge density at a given ion is summed over all the wave numbers in the Fermi sphere it gives the positive charge distribution known as orthogonalization hole. The orthogonallization hole potential is involved in the energy dependent component vqf and WR of the form factor through the core shift fnl. Originally Harrison (1966) has taken vopw without any reduction i.e. $\beta=1$. Later he has suggested $\beta = 5/8$ because he has shown that the previous estimate of vopw is 8/5 times higher. Both these choices have been considered.

It is has been observed that except in the range $n \leq 0.2$, the form factors with $\beta=5/8$ are larger than that with $\beta=1$ in respect of magnitude. For C eigenvalue $\lambda=0.88$ and $T_C=45.7$ with $\beta=5/8$ while it is 0.78 and 36.1 respectively with $\beta=1$. For H eigenvalues $\lambda=0.84$ and $T_C=41.98$ with $\beta=5/8$ while it is 0.72 and 30.2 respectively with $\beta=1$.

Hence $\beta$=5/8 increases both $\lambda$ and $T_C$. A suitable combination of $\alpha$ and $\beta$ is therefore necessary to get reasonably agreement of $T_C$.

In chapter V the impact of orthogonalization hole parameter $\beta$ has been studied in respect of the form factor and also $\lambda$ and TC. When the localized charge density at a given ion is summed over all the wave numbers in the Fermi sphere it gives the positive charge distribution known as orthogonalization hole. The orthogonallization hole potential is involved in the energy dependent component vqf and WR of the form factor through the core shift fnl. Originally Harrison (1966) has taken vopw without any reduction i.e. $\beta$=1. Later he has suggested $\beta$ = 5/8 because he has shown that the previous estimate of vopw is 8/5 times higher. Both these choices have been considered.

It is has been observed that except in the range $n \leq 0.2$, the form factors with $\beta$=5/8 are larger than that with $\beta$=1 in respect of magnitude. For C eigenvalue $\lambda$=0.88 and TC=45.7 with $\beta$=5/8 while it is 0.78 and 36.1 respectively with $\beta$=1. For H eigenvalues $\lambda$=0.84 and TC=41.98 with $\beta$=5/8 while it is 0.72 and 30.2 respectively with $\beta$=1.

Hence $\beta$=5/8 increases both $\lambda$ and TC. A suitable combination of $\alpha$ and $\beta$ is therefore necessary to get reasonably agreement of $T_C$.

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