Pseudopotential approach to superconductivity in MgB$_2$

K S Sharma$^1$, Nidhi Bhargava$^1$, Ritu Jain$^1$, Varsha Goyal$^1$, Ritu Sharma$^2$ & Smita Sharma$^3$

$^1$International College for Girls (Autonomous), The IIS University, Mansarovar, Jaipur 302 020

$^2$Department of Electronics, Malviya National Institute of Technology, Jaipur 302 017

$^3$Department of Physics, Dungar College, Bikaner 334 003

E-mail: smita_sharma_bkn@yahoo.com

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Superconductivity in MgB$_2$ has been re-examined in BCS-Eliashberg framework by employing Mc-Millan’s [Phys Rev, 167 (1968) 331] $T_c$-equation and form factors of MgB$_2$ computed from the form factors of component metals (Model-I). The empty core model pseudopotential due to Ashcroft [Phys Lett, 23 (1966) 48] and random phase approximation form of dielectric screening due to Gellmann and Brueckner [Phys Rev, 106 (1958) 364] are used in the present work. An excellent agreement between the present values and other theoretically computed values of $T_c$ and with the relevant experimental data for MgB$_2$ confirms the validity of the present approach. The explicit dependence of $\lambda$ and $T_c$ on the isotopic masses of Mg and B, as revealed from the present work, confirms the role of lattice vibrations in the superconducting behaviour of MgB$_2$ and the high value of $T_c$ in it may be attributed to the phonon mediated e-e interaction coupled with higher values of phonon frequencies due to light mass of B atoms. It has also been observed that the pseudo-atom model (Model-II) with appropriate choice of the potential parameter $r_e$ successfully explains high value of $T_c$ and isotope effect in MgB$_2$, confirming the prominent role played by electron-phonon interaction in the high-$T_c$ superconductivity observed in MgB$_2$. The isotope effect exponent $\alpha$-values obtained from the two models are in complete agreement with each other and the present value $\alpha = 0.46$ is also much closer to the BCS value of 0.5. Interaction strength $N_0V$ values obtained from the two models are also in perfect agreement with each other and the present value $N_0V = 0.48$ suggests that MgB$_2$ is a strong coupling superconductor.

**Keywords:** Superconductivity, Pseudopotential, Transition temperature, Isotope effect, Electron-phonon interaction

1 Introduction

Following the discovery of superconductivity in MgB$_2$ by Nagamatsu et al.$^1$, a large number of experimental and theoretical researches have been made on this intermetallic compound and its alloys motivated by the fact that it has a record high transition temperature ($T_c$) at 39 K in the hitherto known binary intermetallic superconductors.

Theoretical efforts to explain superconductivity in MgB$_2$ with $T_c$ as high as 39K may be categorized as: (1) Extension of BCS theory of low temperature superconductors to higher temperature domain, and (2) extension of the theories of high $T_c$ cuprates, such as hole superconductivity formulation, to lower temperature domain. In BCS model the superconductivity in the low temperature domain is a consequence of electron-phonon interaction, responsible for electron pairing and long range Bose-Einstein condensation of super-pairs. Coupling of electrons through lattice vibrations or phonons in MgB$_2$ is supported by the presence of boron isotope effect in it$^2-4$. Tunneling experiments as well as theoretical estimation$^5$ of density of states, $N(0)$, also predict presence of energy band gap, $\Delta_0$, in MgB$_2$ such that $2\Delta_0/k_BT_c = 3.9$ ($k_B$ being the Boltzmann’s constant), which is slightly higher than the BCS value of 3.52, an essential characteristic of BCS type superconductors. Since the Fermi surface has two $\sigma$ and two $\pi$ sheets, one might expect anisotropic pairing with different gaps on different sheets.

Kortus et al.$^6$ found that the fortunate combination of strong bonding, reasonable density of states, $N(0)$, at the Fermi level and high phonon frequency is responsible for the high transition temperature in this compound. Kong et al.$^5$ concluded that the unexpected high $T_c$ in MgB$_2$ is due to the large value of electron-phonon coupling strength ($\lambda$) caused by the presence of holes in the B-B bonding $\sigma$ band and the relative softness of the optical bond stretching modes. They categorized MgB$_2$ as an intermediate coupling electron-phonon pairing $s$-wave superconductor. An and Pickett$^7$ consider MgB$_2$ to be a conventional BCS strong coupling $s$-wave electron-phonon pairing superconductor and its high $T_c$ due to (i) hole doping of the covalent $\sigma$ bonds, arising through the ionic and layered character of MgB$_2$, (ii)
2D character of \( \sigma \) band density of states and (iii) an ultra strong deformation potential of the \( \sigma \) bands from the bond stretching modes. Important role played by \( E_{2g} \) phonons in electron-phonon interaction was realized by them. Yildirim et al.\(^8\) observed that a giant anharmonicity in the in-plane boron phonons with \( E_{2g} \) symmetry near the zone centre and non-linear electron-phonon coupling is the key to quantitatively explaining the observed high \( T_c \) and boron isotope effect in MgB\(_2\).

On the other hand Alexandrov\(^9\) observed that the remarkably low value of Fermi energy (\( E_F \)) and the strong coupling of carriers with high frequency phonons are the possible causes of high \( T_c \) in MgB\(_2\), which may be considered to be in non adiabatic regime like cuprates, where Migdal-Eliashberg theory is inappropiate. Cappelluti et al.\(^10\) also observed that high \( T_c \) superconductivity in MgB\(_2\) is mainly driven by \( \sigma \) band states. The peculiar feature of such bands is the smallness of the Fermi energy, which induces non-adiabatic channels of electron-phonon interaction.

Varshney et al.\(^11\) on the basis of an effective two dimensional dynamic interaction potential incorporating the screening of holes as carriers by charge density fluctuations and optical phonons observe that superconductivity in MgB\(_2\) is due to hole carriers in strong coupling regime.

Most of the theoretical investigations of superconductivity in MgB\(_2\) using electron-phonon interaction are either based on the solution of Eliashberg gap equations in isotropic as well as anisotropic forms or by using McMillan’s \( T_c \)-equation either in its original form or in the modified form given by Allen and Dynes\(^12\) to obtain electron-phonon coupling strength (\( \lambda \)) from the experimental values of \( T_c \), however there is hardly any work in which the electron-phonon coupling strength (\( \lambda \)) has been quantitatively estimated from the spectral function \( \alpha^2(\omega)F(\omega) \), where \( \alpha^2(\omega) \) is called the electron-phonon coupling function and \( F(\omega) \) is the phonon density of states, or by using the electron-ion interaction expressed in the form of a pseudopotential.

In the present study, the well established pseudopotential methodology based on BCS-Eliashberg-McMillan framework is used, in which the material properties like electron-phonon coupling strength (\( \lambda \)) and Coulomb pseudopotential (\( \mu^* \)) are obtained from the knowledge of electron-ion pseudopotential, dielectric screening and phonon spectrum. Since only those phonons are useful for electron-phonon interaction leading to superconducting state, which can exchange energy and momentum with the electrons having energy between \( (E_F - \hbar \omega) \) and \( (E_F + \hbar \omega) \), whole of the phonon spectrum is not required. It is, therefore, replaced by the use of a most representative phonon frequency, which is generally taken as the average square phonon frequency \( <\omega^2> \). The superconducting state properties like transition temperature (\( T_c \)) isotope effect exponent (\( \alpha \)) and effective interaction strength (\( N_0V \)) are then obtained by using the values of \( \lambda \), \( \mu^* \), average square phonon frequency \( <\omega^2> \) and isotopic mass (\( M \)) relevant to the superconductor. This approach has been successfully used in the past for metallic superconductors, superconducting alloys and metallic glasses\(^13\). In the present study Ashcroft’s empty core model pseudopotential has been used for the sake of simplicity and RPA form of dielectric screening due to Gellman and Brueckner is employed which takes care of exchange and correlation effects of the electron gas through band mass (\( m_b \)), explicitly involved in this screening. The relevant expressions of the model pseudopotential and dielectric screening have been used by Sharma et al.\(^13\), who found them to work well in explaining superconductivity in metals, alloys and metallic glasses.

### 2 Theory

McMillan is followed in defining electron phonon coupling strength by\(^13\):

\[
\lambda = 2 \int_0^\infty d\omega \alpha^2(\omega) F(\omega) / \omega \quad \ldots (1)
\]

The spectral function, \( \alpha^2(\omega) F(\omega) \), when appropriately evaluated in the plane-wave approximation for scattering on the Fermi surface, yields:

\[
\lambda = \frac{m^*}{4\pi^2 k_F M N} <\omega^2> \int_0^{2k_F} dq |V^S(q)|^2 \quad \ldots (2)
\]

where \( \tilde{q} \) is the change in electron wave vector \( \tilde{k} \) in scattering on the Fermi-surface, \( m^* \) is the effective mass of electron, \( M \) is the ionic mass, \( N \) is the ion number density and \( k_F \) is the Fermi radius of the system under consideration and

\[
V^S(q) = \langle \tilde{k} + \tilde{q} | V | \tilde{k} > l \in (q) \quad \ldots (3)
\]
represents the screened atomic form factors, where \( \epsilon(q) \) is the dielectric screening function and \(<\tilde{k} + \tilde{q}|V|\tilde{k}>\) is the matrix element for the electron scattering from state \(|\tilde{k}>\) to state \(|\tilde{k} + \tilde{q}>)\) on the Fermi surface, also called the ‘bare ion potential’. In Eq. (3) \(|\tilde{k}>\) represents the conduction band states normalized over the crystal volume (\(\Omega\)), also called as a ‘ket’ vector in Dirac notation and is given by:

\[
|\tilde{k}> = \Omega^{-1/2} e^{i\tilde{k}\cdot\tilde{r}} \quad \ldots (4)
\]

whereas \(<\tilde{k} + \tilde{q}|\) the complex conjugate transpose of the ket state \(|\tilde{k} + \tilde{q}>\), called as a ‘bra’ vector in Dirac notation is given by:

\[
<\tilde{k} + \tilde{q}| = \Omega^{-1/2} e^{-i\tilde{k}\cdot\tilde{r}} \quad \ldots (5)
\]

As such, an expression for the matrix element may be written as:

\[
<\tilde{k} + \tilde{q}|V|\tilde{k}> = \Omega^{-1} \int_{\Omega} e^{-i\tilde{k}\cdot\tilde{r}} V(r) e^{i\tilde{k}\cdot\tilde{r}} d\Omega \quad \ldots (6)
\]

As apparent from above, here the integration is over the volume of the crystal.

On using

\[
x = \frac{q}{2k_F} \quad \text{and} \quad N^{-1} = \Omega_0 = \frac{3\pi^2 z^*}{k_F^3},
\]

one obtains from Eq. (2)

\[
\lambda = \frac{12 m^* z^*}{M} \int_0^1 dx x^3 |V(x)|^2 \quad \ldots (7)
\]

where \(\Omega_0\) represents atomic volume and \(z^*\) is the effective valence of ions, which is related to the valency \(z\) of the corresponding metallic ions by:

\[
z^* = (2 - m_E) z \quad \ldots (8)
\]

where \(m_E\) is the component of the effective mass \(m^*\) of the electron, taking in to account the non-locality in energy and related to the effective mass \(m^*\) by:

\[
m^* = m_E x m_K.
\]

Here \(m_K\) is the momentum dependent component of \(m^*\).

The repulsive interaction between electrons in a superconductor is given by the Coulomb pseudopotential \((\mu^*)\), as follows:\(^{13}\):

\[
\mu^* = \frac{m_b}{\pi k_F^2} \int_0^1 dx \frac{1}{x^2} \ln \left[ \frac{k_F^2}{20\theta_D} \int_0^1 dx \right] \quad \ldots (9)
\]

where \(\theta_D\) is the Debye temperature.

The relevant expressions for the transition temperature \((T_c)\) and isotope effect exponent \((\alpha)\) have been obtained by McMillan from the solutions of the Eliashberg gap equations. The same are given\(^{13}\) respectively by:

\[
T_c = \frac{\theta_D}{1.45} \exp \left[ -1.04(1 + \lambda) \left( \frac{\lambda - \mu^*(1 + 0.62\lambda)}{\lambda + \mu^*} \right) \right] \quad \ldots (10)
\]

and

\[
\alpha = \frac{1}{2} \left[ 1 - \left( \frac{\mu^* \ln \left( \frac{\theta_D}{1.45T_c} \right)}{1 + \mu^*} \right)^2 \right] \quad \ldots (11)
\]

and the relevant expression for effective interaction strength \((N_0V)\) has been obtained in the following form:\(^{13}\):

\[
N_0V = \frac{\lambda - \mu^*}{1 + (10/11)\lambda} \quad \ldots (12)
\]

For obtaining screened atomic form factors \(V(x)\) through Eq. (3), empty core model pseudopotential \(V(x)\) due to Ashcroft is used and the dielectric screening function \(\epsilon(x)\) obtained in Random Phase Approximation by Gellmann and Brueckner, which have been found to work well in explaining the superconducting state in binary alloys and metallic glasses\(^ {13}\) are given respectively by:

\[
V(x) = \frac{\pi z^*}{\Omega_0 x^2 k_F} \cos(2xk_Fr_C) \quad \ldots (13)
\]

and

\[
\epsilon(x) = 1 + \frac{m^*}{\pi k_F x^2} \left[ 0.5 + \frac{(1 - x^2)}{4x} \ln \left( \frac{1 + x}{1 - x} \right) \right] \quad \ldots (14)
\]
where \( r_c \) is the potential parameter, which represents effective atomic core radius, such that in \( r \)-space \( V = 0 \) for \( r < r_c \) and varies as \((1/r)\) for \( r > r_c \). The value of \( r_c \) for a superconductor is obtained by fitting it to some experimental property of the superconductor.

Form factors for \( \text{MgB}_2 \) in the first approach (Model-I) adopted in the present work are obtained from the form factors of component elements Mg and B by employing the relation:

\[
V_{\text{MgB}_2}^S = \frac{1}{3} \left[ V_{\text{Mg}}^S + 2V_{\text{B}}^S \right] \tag{15}
\]

The form factors of \( \text{MgB}_2 \) obtained from Eq. (15) are used in Eq. (7) to obtain \( \lambda \) and after obtaining \( \mu^* \) from Eq. (9), one obtains \( T_c, \alpha \) and \( N_0V \) for \( \text{MgB}_2 \) respectively from Eqs (10)-(12).

Though the Fermi surface of \( \text{MgB}_2 \) is quite complex, the Fermi surfaces of the component elements, i.e., Mg and B, are almost spherical. As such, the methodology of computing form factors of \( \text{MgB}_2 \) from the form factors of component elements is theoretically justified. Another approach (Model-II) to deal with the superconductivity of binary alloys or metallic glasses is to implant pseudo atoms with effective atomic core radius, such that in \( r \)-space.

\[
<T> = \frac{1}{2} \omega_{l} + \omega_{t}
\]

(16)

where \( \omega_{l} \) and \( \omega_{t} \) are respectively the most representative maximum frequencies of longitudinal and transverse modes of the phonon spectrum. In the absence of phonon frequency data \( \omega_{l} \) is set equal to \( \theta_D \) and \( \omega_{t} \) is evaluated from \((C_L/C_V) \theta_D \), where \( C_L \) and \( C_V \) are sound velocities for longitudinal and transverse modes respectively. Another approach is due to Butler, in which case

\[
<T> = 0.69 \theta_D
\]

(17)

The third approach to this problem is due to Known et al., who take

\[
<T> = \frac{1}{\sqrt{2}} \theta_D
\]

(18)

In the computer simulation made in this study, it has been observed that the superconducting state properties of \( \text{MgB}_2 \) are quite sensitive to the phonon frequency, as such an appropriate selection of \( <\omega^2> \) is desirable. We observe that Eqs (16) and (18) overestimate \( <\omega^2> \) resulting in lowering of the values of \( \lambda \) and \( T_c \), as such Eq. (17) is used in the present work, which provides proper estimate of phonon frequencies in \( \text{MgB}_2 \) from its \( \theta_D \).

The Debye temperature (\( \theta_D \)) enters in formulation through \( <\omega^2> \) given by Eq. (17), used in the present work and through Eq. (10), the McMillan’s expression for \( T_c \). As such, the selection of \( \theta_D \) is also very crucial in theoretical explanation of superconductivity in \( \text{MgB}_2 \). The values of \( \theta_D \) reported in literature vary from 700 to 1016 K. In the computer simulation made, it has been observed that higher values of \( \theta_D \) lower down the value of electron phonon coupling strength (\( \lambda \)), which overpowers the advantage of the pre-factor \( \theta_D/1.45 \) in Eq. (10) and results in a net decrease in \( T_c \) value. The value \( \theta_D = 700 \) K, reported by Known et al., has been found to be quite appropriate for theoretical explanation of superconductivity in \( \text{MgB}_2 \) and as such this value of \( \theta_D \) is used in the present work.

3 Results and Discussion

Phonon frequency has an important role in explaining the behaviour of a superconductor through appearance of \( <\omega^2> \) in the expression of \( \lambda \), which could be obtained from the phonon band structure of the system. An alternative empirical method is used for the sake of simplicity, for which three types of approaches are available in literature. The first approach is due to Allen and Cohen in which case:

\[
<\omega^2> = \frac{\omega_{l} + \omega_{t}}{2}
\]

(16)

where \( \omega_{l} \) and \( \omega_{t} \) are respectively the most representative maximum frequencies of longitudinal and transverse modes of the phonon spectrum.
For atomic mass \((M)\), average isotopic masses of Mg and B are used, the values of which as reported in the literature are 24.312 and 10.811 amu respectively.

The values of other input parameters used in this work have been presented in Table 1. Since the values of \(m^*\), \(m_b\) and \(m_E\) for B are not available in literature, relevant values of Al are used, which belongs to the same group as B. In pseudo-atom model (Model-II) the relevant values of parameters for MgB\(_2\), except for \(r_c\) and \(\theta_D\), are obtained from the values of such parameters for Mg and B by using the Vegard’s rule\(^{13}\) in the following form:

\[
p_{\text{MgB}_2} = \frac{1}{3} \left( p_{\text{Mg}} + 2 p_{\text{B}} \right)
\]

... (19)

where \(p\) represents a parameter\(^{16}\). For \(\theta_D\) of MgB\(_2\) experimental value \(\theta_D = 700\)K is used for reasons as discussed above. The same value of \(\theta_D\) is also used for obtaining \(<\omega^2>\) for MgB\(_2\) from Eq. (17). The \(<\omega^2>\) values for the component metals, i.e. Mg and B, given in Table 1 are also based on Eq. (17). In Model-I, the relevant values of potential parameter \(r_c\) for component metals are obtained by fitting it to the form factors of the respective elements. The form factors of component elements so obtained are used in Eq. (15) to obtain form factors of MgB\(_2\).

In pseudo-atom model (Model-II), the value of potential parameter \(r_c\) is obtained by fitting it to the form factors of MgB\(_2\) obtained from Model-I. Thus in Model-II \(r_c = 1.515\) is obtained, for which the form factors are pictorially shown in Fig. 1.

The values of superconducting state parameters, viz. \(\lambda\), \(\mu^*\), \(T_c\), \(\alpha\) and \(N_0V\) of MgB\(_2\) obtained from the two approaches, i.e., first by computation of form factors of MgB\(_2\) from the relevant values for component metals through Eq. (15) (i.e., Model-I), and secondly by using the pseudo atom approach (i.e., Model-II) for \(r_c = 1.515\), have been presented in Table 2 along with relevant experimental data and other values obtained in some important theoretical investigations.

It may be observed from Table 2 that the values of superconducting state parameters obtained from the two approaches are in perfect agreement with each other. The \(T_c\) values calculated in this paper show excellent agreement with the experimental \(T_c\) value of 39 K by Nagamatsu et al.\(^{1}\), 39.25 K by Tomita et al.\(^{17}\) and 39.2 K due to Osborn et al.\(^{18}\). Some of the other reported theoretical results of \(T_c\) have been given in the last column of Table 2. It may be observed that the theoretically computed values of 39 K by Choi et al.\(^{19}\) and 39.4 K by Balaselvi et al.\(^{20}\) are also in good agreement with the present results. The present \(T_c\) values are also well within the limit 37 to 42 K set by Choi et al.\(^{19}\).

The present values of \(\lambda\) also show good agreement with the value 0.9 reported by Osborn et al.\(^{18}\) on the basis of inelastic neutron scattering measurements.

<table>
<thead>
<tr>
<th>Table 1 — Input parameters</th>
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<td>Parameter</td>
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<td>(z^*)</td>
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<td>(M) (amu)</td>
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<tr>
<td>(\theta_D) (K)</td>
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<td>(&lt;\omega^2&gt;\times10^5) (K(^2))</td>
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</table>

![Fig. 1 — Form factors of MgB\(_2\) obtained from pseudo-atom model (Model-II)](image-url)
The experimental value of $\lambda$ reported by Kortus et al.\textsuperscript{6} to be 1.4 is on the higher side, whereas $\lambda = 0.75$ reported by An and Pickett\textsuperscript{7} on the basis of specific heat measurements is some what on the lower side. Whereas most of the theoretical results for $\lambda$ given in the last column of Table 2 show good agreement with the present results, the value $\lambda = 1.08$ obtained by Knigavko and Marsinglio\textsuperscript{4} is in the best agreement. Also the $\lambda$ values of 0.907 and 0.922 reported respectively for Mg\textsuperscript{10}B\textsubscript{2} and Mg\textsuperscript{11}B\textsubscript{2} by Yildirim et al.\textsuperscript{8} are in good agreement with the present values of $\lambda$. It may be observed that present $\lambda$ values for MgB\textsubscript{2} are also well within the limit 0.65 to 1.2 prescribed by Hinks et al.\textsuperscript{3}.

The same value $\mu^* = 0.124$ is obtained by us from the two approaches in the present formulation, which shows a good agreement with the value 0.12 reported by Choi et al.\textsuperscript{19} and lie well within the range 0.10 to 0.14 prescribed by Choi et al.\textsuperscript{19} on the basis of anisotropic Eliashberg equation including anharmonicity in the phonon frequencies.

The present formulation for the isotope effect exponent provides $\alpha = 0.46$ from both the models. This value is closer to the BCS value of 0.5 as compared to experimental values, $\alpha_0 = 0.26$ due to Bud’ko et al.\textsuperscript{2} and $\alpha_0 = 0.30$ and $\alpha_{\text{Mg}} = 0.02$ (i.e. $\alpha_{\text{total}} = 0.32$) due to Hinks et al.\textsuperscript{3}. Some of the theoretical results for $\alpha$ values of MgB\textsubscript{2} have been given in the last column of Table 2. It may be observed that $\alpha_{\text{total}} = 0.36$ and 0.50 predicted respectively by Choi et al.\textsuperscript{19} and Osborn et al.\textsuperscript{18} are quite close to the present value $\alpha = 0.46$. The fact that the present $\alpha$ values from both the approaches show an excellent agreement with the value $\alpha_0 = 0.46$ obtained by Kong et al.\textsuperscript{5} and being also quite close to the BCS value of 0.5, re-affirms that the origin of superconductivity in MgB\textsubscript{2} may be attributed to the electron-phonon coupling.

In the absence of other values of interaction strength, an effective comparison of the present values of $N_0V$ could not be possible, however the same value $N_0V = 0.48$ obtained by us from both the approaches confirms the validity of present formulation and reveals that MgB\textsubscript{2} is a strong coupling superconductor in conformity with the observations of Kong et al.\textsuperscript{3}, Kortus et al.\textsuperscript{6}, Yildirim et al.\textsuperscript{8} and Osborn et al.\textsuperscript{18}.

The presence of isotope effect in MgB\textsubscript{2} confirms the role of electron-phonon interaction or electron-lattice interaction in the origin of superconductivity in it. In order to make this aspect more explicit, dependence of $\lambda$ and $T_c$ on isotopic mass of Mg and B is investigated. For this purpose two isotopes of Boron, i.e. $^{10}$B and $^{11}$B with atomic mass 10.0051 and 10.9952 amu respectively\textsuperscript{3} and three isotopes of Mg: $^{24}$Mg, $^{25}$Mg, and $^{26}$Mg with masses 23.985042, 24.985837 and 25.982593 amu, respectively are used. In this analysis three other isotopic masses of Mg used by Hinks et al.\textsuperscript{3} for $^{24}$Mg, $^{25}$Mg and natural Magnesium i.e. 24.001, 25.001 and 24.305 amu, respectively are also included. The dependence of $T_c$ on isotopic mass of Mg and B for the two models has been shown in Fig. 2. The slope of the linear graphs for $T_c$ clearly depicts the dependence of $T_c$ on isotopic mass of Mg and the separation between the $T_c$ lines for $^{10}$B and $^{11}$B is a measure of the dependence of $T_c$ on isotopic mass of B. Whereas the dependence of $T_c$ on isotopic mass of B is quite prominent, the dependence of $T_c$ on isotopic mass of Mg is also clearly visible from the slope of the
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$T_c$-graphs, which is now much better than that obtained by Hinks et al.$^3$. For Boron isotopes $\delta T_c \sim 2.75$ K is obtained in this study from both the models, as against $\delta T_c = 1$ K ($T_c = 39.2$ K for Mg$^{11}$B$_2$ and 40.2 K for Mg$^{10}$B$_2$) measured by Bud’ko et al.$^2$ and $\delta T_c = 1.7$ K calculated by Kong et al.$^5$. Hinks et al.$^3$ measured $\delta T_c \sim 1.16$K for Boron isotope effect in MgB$_2$, whereas Yildirim et al.$^8$ obtained $\delta T_c = 0.8$ K, ($T_c = 39.4$K for Mg$^{10}$B$_2$ and 38.6K for Mg$^{11}$B$_2$). Further, whereas the isotope effect of Mg isotopes on $T_c$ was found to be negligibly small by Hinks et al.$^3$, in the present work $\delta T_c \sim 2.78$ K from the Model-I and $\delta T_c \sim 2.63$ K from the Model-II for mass variation of Mg isotopes are obtained.

The isotope effect for B and Mg isotopes in MgB$_2$ are also clearly visible from Fig. 3, in which $\lambda$ values obtained from the two models (i.e., model-I and model-II) against the isotopic mass of Mg are plotted. Linear curves for the two isotopes of B (i.e., $^{10}$B and $^{11}$B) are obtained. The slope of $\lambda$ curves for each isotope of B clearly depicts the effect of Mg isotopes on $\lambda$, whereas the separation between the two almost parallel $\lambda$-lines is due to the major role played by boron isotopes in electron-phonon coupling. This proves the role of ionic mass and the prominent role played by the boron planes in the superconductivity observed in MgB$_2$.

4 Conclusions

Present studies clearly establish that superconductivity in MgB$_2$ originates from electron-phonon interaction. The B $p_{x,y}$ planar orbitals of Boron in MgB$_2$ support electron-phonon interaction and pairing of electrons. In addition to the 2D flow of electron pairs, inter-planar hopping of quasi-particles and their long range cooperative phenomenon provides them with a 3D character. The present investigations prove that BCS-Eliashberg-McMillan formulation with model pseudopotential approach successfully explains superconductivity in MgB$_2$.

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