The effect of interband interactions of phonon and charge fluctuation on the superconducting parameters of MgB$_2$

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Abstract
We have investigated the effect of an unconventional pairing mechanism in MgB$_2$ using a two-band model within the framework of Bogoliubov–Valatin formalism. The approach incorporates the intraband s-wave interaction in the s- and p-bands, as well as interband s-wave interaction between them. The analysis assumes that the pairing interaction matrix comprises of attractive electron–phonon, charge fluctuation and repulsive electron–electron (Coulomb) interactions to account for superconductivity in MgB$_2$. The model is used to estimate the transition temperature and isotope effect exponent as well as to elucidate the importance of interband contributions in the superconductivity of the system

(Some figures in this article are in colour only in the electronic version)

1. Introduction

The discovery of superconductivity in magnesium diboride, MgB$_2$, at a transition temperature, $T_c \sim 39$ K [1] has attracted a lot of attention both theoretically and experimentally in the field of condensed matter physics. This intermetallic material was associated with conventional superconductors based on pairing by electron–phonon coupling but its remarkably high-$T_c$ [2] cannot be explained using the conventional (Bardeen–Copper–Schrieffer (BCS)) theory [3]. Also, the experimentally [4, 5] observed shift in the isotope exponent reveals the importance of phonon contribution to the $T_c$.

Electronic band structure calculation [6, 7] predicted the existence of two-dimensional (2D) covalent in-plane (σ-band) and three-dimensional (3D) metallic type inter-layer (π-band) conducting bands at the Fermi level, $E_F$ for this system. The σ-band is strongly coupled with phonons within the honeycombed boron layer while electrons in the π-band can support only weak coupling.

The multi-band gap nature of superconductivity in MgB$_2$ was first predicted theoretically by Liu et al [8] and has been observed in various experiments such as: tunneling spectroscopy [9, 10], point-contact spectroscopy [11], specific heat measurements [12] and magneto-Raman spectroscopy [13]. The two-band nature of superconductivity in MgB$_2$ is already well established [14] and the BCS mechanism has been supported by photoemission spectroscopy [15] and scanning tunneling microscopy [16] among others. Also, the specific heat analysis performed by Wälte et al [17] has revealed the weak interband coupling scenario in MgB$_2$ and they showed that the data are best explain within the two-band BCS theory of superconductivity.

Choi et al [18] used the Eliashberg formalism to show that the σ-bonding states possess an average energy gap of 6.8 meV while the π-states have weak pairs with an average energy gap of 1.8 meV. Pickett [19] explained the double gap as having two transition temperatures, one at 45 K ($\Delta_\sigma$) and the other at 15 K ($\Delta_\pi$), which result in a transition temperature (for the bulk material) of 39 K [1]. Putti et al [20] and Nicol and Carbotte [21] provided a good illustration of how the two-bands integrate to result in a single $T_c$ due to strong interband processes. That is, the two-gaps merge to one isotropic BCS gap [22] and possess one critical temperature as a result of strong interband scattering [8, 20, 21, 23]. However, the merging of the two-bands does not result in the superconducting properties of a one-band superconductor because of the presence of strong anisotropy coupling as well as both intra and interband scattering that affect the superconducting properties [21, 20].
In MgB$_2$, the boron isotope exponent, $\beta(B)$ is only significant while the Mg isotope exponent, $\beta(Mg)$ is small but non-zero. Budko et al. [4] measured $\beta(B) = 0.26$ and the same value was recently obtained by Broto et al. [24]. Hinks et al. [5] measured $\beta(B)$ to be 0.30 and $\beta(Mg)$ to be 0.02, resulting in a total isotope exponent, $\beta$, equals 0.32 for MgB$_2$. Ord et al. [25] calculated $\beta = 0.34$ using electron–phonon and Coulomb interactions in the $\sigma$-bands as well as the interband scattering of intraband pairs within a two-band model. Choi et al. [26] have calculated $\beta(B) = 0.32$ and $\beta(Mg) = 0.03$ using isotropic Eliashberg theory. Also, Calandra’s group [27] found that inclusion of strong electron–phonon coupling and the Coulomb repulsion effect in the one-band or two-band Migdal–Eliashberg approach suppress the isotope exponent of boron, $\beta(B)$, to a value of about 0.4–0.45. Studies have suggested that the low isotope effect is mainly due to phonon anharmonicity [28] and interband Coulomb repulsion [25, 29].

Despite the fact that the isotope effect experiment supports the phonon mediated BCS type superconductor, the observed small value of $\beta$ cannot be explained by the conventional BCS theory [3]. Also, large amounts of effort devoted to the study of this phenomenon have not provided a clear understanding of the reduced isotope effect [27] and the pairing mechanism [2].

Among the nonconventional models that have been proposed for explaining the superconductivity in MgB$_2$ are the electronic mechanism mediated by collective excitation pairing [30, 31], bipolarons [32] and the electronic resonance-valence-bond (RVB) model [33].

Ku et al. [34] showed that the presence of collective excitations, consisting of coherent charge fluctuation between Mg and B sheets affects the optical properties of the material. Shortly after discovery, electron energy-loss spectroscopy (EELS) [35, 36] suggested that a special electronic contribution may affect the superconductivity of MgB$_2$. First principle calculation predicted that the excitations arise from interband transitions in MgB$_2$ [30]. Combined EELS and ab initio calculations of the plasmon structure in MgB$_2$ have shown a peak at 2.4 eV and several peaks for higher energies [37]. Optical experiment [38] revealed that the intense peak is due to the transition from the $\sigma$- to the $\pi$-band. The optical study went further to suggest that these collective electronic modes affect the color of MgB$_2$. That is, polarization of light is bluish silver for $E \parallel ab$ and yellow for $E \parallel c$. Another optical experiment suggested that the multi-band picture is necessary to understand the optical spectra of MgB$_2$ [39].

First principles calculations of the excitation spectra in MgB$_2$ involving all the three symmetry momentum directions have confirmed the existence of the long-lived collective excitations and its presence in the region of optical frequencies strongly affects the optical properties [40]. Recently, Silkin et al. [41] demonstrated that the unknown long-lived collective mode corresponds to coherent charge fluctuations between the boron $\sigma$- and $\pi$-band ($\sigma\pi$ mode) as well as having a periodic sine-like dispersion for energies below 0.5 eV. Varshney and Nagar [42] have employed a model involving collective charge fluctuation, within the Eliashberg formalism, to calculate some superconducting parameters of MgB$_2$ without the inclusion of interband interactions.

The present study is motivated by the predictions of collective coherent charge fluctuation from first principles calculations [30, 34, 40, 41], EELS [35, 36] and optical [38, 39] experiments as well as the fact that MgB$_2$ is conclusively agreed to be a two-band BCS type superconductor with exceptionally high $T_c$ (see reviews, [2, 14]). Therefore, we employ the two-band BCS model within the Bogoliubov–Valatin formalism and naively assume that the pairing interaction matrix comprises attractive electron–photon, repulsive Coulomb and attractive electron–plasmon interactions to study the superconducting parameters of MgB$_2$. This is to elucidate the role of charge fluctuation on the system and the interband contribution to the superconducting properties of MgB$_2$. This kind of pairing mechanism has been used by Tewari and Gumber [43] within the one-band BCS model to study the effect of plasmons on the yttrium and lanthanum based superconductors. The paper is organized as follows; in section 2, we present the model. Then, section 3 will be devoted to results and analysis. Finally, section 4 is the conclusion.

2. Model

In accord with the original formulation by Suhl et al. [45], on two-band superconductivity, and more recently, studies on the two-band model of MgB$_2$ superconductor [29, 46, 47], the effective Hamiltonian of the system can be written as:

$$H = \sum_{iks} \epsilon_{ik} c_{ik}^\dagger c_{iks} + \sum_{ikk'} V_{ikk'} c_{ik}^\dagger c_{-i-k'}^\dagger c_{-i-k} c_{ik}$$

$$+ \sum_{kk'} V_{\pi\pi k} c_{\pi k}^\dagger c_{-\pi-k}^\dagger c_{-\pi-k'} c_{\pi k'}$$

$$+ \sum_{kk'} V_{\sigma\sigma k} c_{\sigma k}^\dagger c_{-\sigma-k}^\dagger c_{-\sigma-k'} c_{\sigma k'}$$

(1)

where $\epsilon_{ik}$ are kinetic energies of the two ($i = \pi, \sigma$) bands measured relative to the Fermi level, $k(k')$ is the Bloch wavevector, $V_{ikk'}$ are the intraband potential matrices, $s$ is spin index, $\dagger$ ($\downarrow$), $c_{iks}$ ($c_{jk}$) are the creation (annihilation) operators, for the $i$th-band, and $V_{\pi\pi k}$ is the interband interaction. Employing the standard Bogoliubov–Valatin transformation [48, 49] in equation (1), the linearized gap equations ($T_c$ equation) can be written as:

$$\Delta_{\pi k} = -\sum_{k'} V_{\pi k} \frac{\Delta_{k'}}{2\epsilon_{k'}} (1 - 2f(\epsilon_{k'}))$$

$$- \sum_{k'} V_{\pi k} \frac{\Delta_{k'}}{2\epsilon_{k'}} (1 - 2f(\epsilon_{k}))$$

(2)

$$\Delta_{\sigma k} = -\sum_{k'} V_{\sigma k} \frac{\Delta_{k'}}{2\epsilon_{k'}} (1 - 2f(\epsilon_{k}))$$

$$- \sum_{k'} V_{\sigma k} \frac{\Delta_{k'}}{2\epsilon_{k'}} (1 - 2f(\epsilon_{k}))$$

(3)

where $\Delta_{ik}$ are the gap parameters for two-bands, $\pi$ and $\sigma$, $f(\epsilon_{ik})$ are the Fermi–Dirac occupation number for quasiparticle states to energies $\epsilon_{ik}$ above the Fermi level.

In the present model, we shall assume the pairing interaction matrices ($V_{ikk'}$) are made up of contributions from the attractive electron–photon–phonon ($V_{ph}$), repulsive electron–electron
\(\Delta_{\pi k} = -N(0) \int (-V_{\pi ph} + V_{\pi c} - V_{\pi pl}) \times \frac{\Delta_{\sigma k}}{2\epsilon_{\sigma k'}}(1 - 2f(\epsilon_{\sigma k'})) d\epsilon_{\sigma k'} \)

\(-N(0) \int (-V_{\pi ph} + V_{\pi c} - V_{\pi pl}) \times \frac{\Delta_{\sigma k}}{2\epsilon_{\sigma k'}}(1 - 2f(\epsilon_{\sigma k'})) d\epsilon_{\sigma k'} \)

\(-N(0) \int (-V_{\pi ph} + V_{\pi c} - V_{\pi pl}) \times \frac{\Delta_{\sigma k}}{2\epsilon_{\sigma k'}}(1 - 2f(\epsilon_{\sigma k'})) d\epsilon_{\sigma k'}

\Delta_{\pi k} = -N(0) \int (-V_{\pi ph} + V_{\pi c} - V_{\pi pl}) \times \frac{\Delta_{\sigma k}}{2\epsilon_{\sigma k'}}(1 - 2f(\epsilon_{\sigma k'})) d\epsilon_{\sigma k'}

\(\Delta_{\pi c} = -N(0) V_{\pi ph} \int_{-\omega_{ph}}^{\omega_{ph}} \Delta_{\pi ph} \frac{(1 - 2f(\epsilon_{\sigma k'}))}{2\epsilon_{\sigma k'}} d\epsilon_{\sigma k'} + N(0) V_{\pi pl} \int_{-\omega_{pl}}^{\omega_{pl}} \Delta_{\pi pl} \frac{(1 - 2f(\epsilon_{\sigma k'}))}{2\epsilon_{\sigma k'}} d\epsilon_{\sigma k'}

\(\Delta_{\pi c} = -N(0) V_{\pi c} \left( \int_{-\omega_{c}}^{\omega_{c}} \Delta_{\pi c} + \int_{-\omega_{c}}^{\omega_{c}} \Delta_{\pi ph} + \int_{-\omega_{c}}^{\omega_{c}} \Delta_{\pi pl} \right) \quad (\text{for } \sigma = \pi)

\(\Delta_{\pi c} = -N(0) V_{\pi c} \left( \int_{-\omega_{c}}^{\omega_{c}} \Delta_{\pi c} + \int_{-\omega_{c}}^{\omega_{c}} \Delta_{\pi ph} + \int_{-\omega_{c}}^{\omega_{c}} \Delta_{\pi pl} \right) \quad (\text{for } \sigma = \pi)

\(\Delta_{\pi c} = -N(0) V_{\pi c} \left( \int_{-\omega_{c}}^{\omega_{c}} \Delta_{\pi c} + \int_{-\omega_{c}}^{\omega_{c}} \Delta_{\pi ph} + \int_{-\omega_{c}}^{\omega_{c}} \Delta_{\pi pl} \right) \quad (\text{for } \sigma = \pi)

\(\Delta_{\pi c} = -N(0) V_{\pi c} \left( \int_{-\omega_{c}}^{\omega_{c}} \Delta_{\pi c} + \int_{-\omega_{c}}^{\omega_{c}} \Delta_{\pi ph} + \int_{-\omega_{c}}^{\omega_{c}} \Delta_{\pi pl} \right) \quad (\text{for } \sigma = \pi)

\(\Delta_{\pi c} = -N(0) V_{\pi c} \left( \int_{-\omega_{c}}^{\omega_{c}} \Delta_{\pi c} + \int_{-\omega_{c}}^{\omega_{c}} \Delta_{\pi ph} + \int_{-\omega_{c}}^{\omega_{c}} \Delta_{\pi pl} \right) \quad (\text{for } \sigma = \pi)

\(\Delta_{\pi c} = -N(0) V_{\pi c} \left( \int_{-\omega_{c}}^{\omega_{c}} \Delta_{\pi c} + \int_{-\omega_{c}}^{\omega_{c}} \Delta_{\pi ph} + \int_{-\omega_{c}}^{\omega_{c}} \Delta_{\pi pl} \right) \quad (\text{for } \sigma = \pi)

\(\Delta_{\pi c} = -N(0) V_{\pi c} \left( \int_{-\omega_{c}}^{\omega_{c}} \Delta_{\pi c} + \int_{-\omega_{c}}^{\omega_{c}} \Delta_{\pi ph} + \int_{-\omega_{c}}^{\omega_{c}} \Delta_{\pi pl} \right) \quad (\text{for } \sigma = \pi)

\(\Delta_{\pi c} = -N(0) V_{\pi c} \left( \int_{-\omega_{c}}^{\omega_{c}} \Delta_{\pi c} + \int_{-\omega_{c}}^{\omega_{c}} \Delta_{\pi ph} + \int_{-\omega_{c}}^{\omega_{c}} \Delta_{\pi pl} \right) \quad (\text{for } \sigma = \pi)

\(\Delta_{\pi c} = -N(0) V_{\pi c} \left( \int_{-\omega_{c}}^{\omega_{c}} \Delta_{\pi c} + \int_{-\omega_{c}}^{\omega_{c}} \Delta_{\pi ph} + \int_{-\omega_{c}}^{\omega_{c}} \Delta_{\pi pl} \right) \quad (\text{for } \sigma = \pi)

\(\Delta_{\pi c} = -N(0) V_{\pi c} \left( \int_{-\omega_{c}}^{\omega_{c}} \Delta_{\pi c} + \int_{-\omega_{c}}^{\omega_{c}} \Delta_{\pi ph} + \int_{-\omega_{c}}^{\omega_{c}} \Delta_{\pi pl} \right) \quad (\text{for } \sigma = \pi)

\(\Delta_{\pi c} = -N(0) V_{\pi c} \left( \int_{-\omega_{c}}^{\omega_{c}} \Delta_{\pi c} + \int_{-\omega_{c}}^{\omega_{c}} \Delta_{\pi ph} + \int_{-\omega_{c}}^{\omega_{c}} \Delta_{\pi pl} \right) \quad (\text{for } \sigma = \pi)

\(\Delta_{\pi c} = -N(0) V_{\pi c} \left( \int_{-\omega_{c}}^{\omega_{c}} \Delta_{\pi c} + \int_{-\omega_{c}}^{\omega_{c}} \Delta_{\pi ph} + \int_{-\omega_{c}}^{\omega_{c}} \Delta_{\pi pl} \right) \quad (\text{for } \sigma = \pi)

\(\Delta_{\pi c} = -N(0) V_{\pi c} \left( \int_{-\omega_{c}}^{\omega_{c}} \Delta_{\pi c} + \int_{-\omega_{c}}^{\omega_{c}} \Delta_{\pi ph} + \int_{-\omega_{c}}^{\omega_{c}} \Delta_{\pi pl} \right) \quad (\text{for } \sigma = \pi)

\(\Delta_{\pi c} = -N(0) V_{\pi c} \left( \int_{-\omega_{c}}^{\omega_{c}} \Delta_{\pi c} + \int_{-\omega_{c}}^{\omega_{c}} \Delta_{\pi ph} + \int_{-\omega_{c}}^{\omega_{c}} \Delta_{\pi pl} \right) \quad (\text{for } \sigma = \pi)

\(\Delta_{\pi c} = -N(0) V_{\pi c} \left( \int_{-\omega_{c}}^{\omega_{c}} \Delta_{\pi c} + \int_{-\omega_{c}}^{\omega_{c}} \Delta_{\pi ph} + \int_{-\omega_{c}}^{\omega_{c}} \Delta_{\pi pl} \right) \quad (\text{for } \sigma = \pi)

\(\Delta_{\pi c} = -N(0) V_{\pi c} \left( \int_{-\omega_{c}}^{\omega_{c}} \Delta_{\pi c} + \int_{-\omega_{c}}^{\omega_{c}} \Delta_{\pi ph} + \int_{-\omega_{c}}^{\omega_{c}} \Delta_{\pi pl} \right) \quad (\text{for } \sigma = \pi)

\(\Delta_{\pi c} = -N(0) V_{\pi c} \left( \int_{-\omega_{c}}^{\omega_{c}} \Delta_{\pi c} + \int_{-\omega_{c}}^{\omega_{c}} \Delta_{\pi ph} + \int_{-\omega_{c}}^{\omega_{c}} \Delta_{\pi pl} \right) \quad (\text{for } \sigma = \pi)
λ ignore the contribution of electron–plasmon interaction (two-square-wells can be recovered from equation (16))

The well-known McMillan [52] expression in two-bands and Equation (20) is the expression for the isotope exponent (\(T_\mu\)) which depends on the scaling factor \(Z_3 = \ln(\omega_{ph}/\omega_{pl})\). Although this can be seen as a crude approximation, we are encouraged by the common belief that the effects of Coulomb screening are drastically reduced by retardation effects due to the different energy scales for electrons and phonons. The effect of Coulombic repulsion is an important concept which is mainly fixed as an adjustable parameter in first principle calculations. A good account of this has been given in [42].

In the present analysis, the electron–phonon and the electron–plasmon cut-off frequencies are \(\omega_{ph} = 812\, K\) [53] and \(\omega_{pl} = 2.2\, eV\) [30], respectively, while the frequency of the Coulomb repulsive parameter \(\omega_c = 750\, meV\) [21]. Assuming an arbitrary total intraband coupling (comprising of electron–phonon and electron–plasmon coupling) \(\lambda + \lambda_{pl} = 0.45\), we estimated the transition temperature, based on equation (16) as 38.80 K for the intra (inter)band Coulomb pseudopotential \(\mu^* = 0.18\) (0.07) and interband parameters of \(\lambda_{\pi\sigma pl} = 0.09\) and \(\lambda_{\pi\sigma} = 0.08\).

Figure 1 shows the variation of Transition temperature \((T_c)\) with interband electron–plasmon interaction \((\lambda_{\pi\sigma pl})\) for different values of \(\mu^*\).

3. Results and discussion

To understand the effect of the assumed pairing mechanism in MgB\(_2\), we proceed to estimate the transition temperature and isotope effect exponent using the available data in the literature. At this point, we have to point out that the repulsive Coulomb coupling parameter is associated with the renormalized Coulomb pseudopotential, \(\mu^* = \frac{\mu}{1 + \lambda_{\pi\sigma pl}}\). The variation of \(T_c\) with \(\lambda_{\pi\sigma pl}\) for the above set of parameters and three different values of \(\mu^*\), that is 0.17, 0.18 and 0.21. This assumed \(\mu^*\) compares well with the Golubov et al [44] values of \(\mu^*_{\pi\sigma} = 0.17\) and \(\mu^*_{\pi\sigma} = 0.21\). It can be observed that \(T_c\) increases with \(\lambda_{\pi\sigma pl}\) but decreases with \(\mu^*\). Also, \(T_c \approx 38.80\, K\) when \(\lambda_{\pi\sigma pl} = 0.09\) for \(\mu^* = 0.18, \mu^*_{\pi\sigma} = 0.07\) and \(\lambda_{\pi\sigma} = 0.08\). And the effective interband coupling, \(\lambda_{\pi\sigma} + \lambda_{\pi\sigma pl} = 0.08 + 0.09 = 0.17\).

Also in figure 1, we can see that \(\lambda_{\pi\sigma pl} = 0\) corresponds to \(T_c \approx 20\, K\) for \(\mu^* = 0.18\), which clearly shows the importance of interband interaction in the high transition temperature of MgB\(_2\).

The variation of \(T_c\) with the interband electron–phonon interaction is shown in figure 2. The lower values of \(\lambda_{\pi\sigma}\) yield unphysical values of \(T_c\) irrespective of \(\mu^*\). The effect of electron–phonon coupling strength on the renormalized repulsive Coulomb parameter, \(\mu^*\) is consistent with the conventional superconductor. This shows that the contribution of interband interactions of phonons and plasmons is crucial in the high-\(T_c\) of MgB\(_2\).

We proceed to analyze the isotope effect of the superconducting MgB\(_2\) based on equation (20). Employing the same parameters used to estimate the transition temperature,
Figure 2. Variation of transition temperature ($T_c$) with interband electron–phonon interaction ($\lambda_{\pi\sigma}$) for different values of $\mu^*$. 

Figure 3. Variation of isotope exponent ($\beta$) with interband electron–phason interaction ($\lambda_{\pi\sigma\text{pl}}$) for different values of $\mu^*$. 

Figure 4. Variation of isotope exponent ($\beta$) with interband electron–phonon interaction ($\lambda_{\pi\sigma}$) for different values of $\mu^*$. 

$T_c \approx 38.80 \text{ K}$, we obtain an exponent, $\beta \approx 0.43$. This is in good agreement with the theoretically calculated values of Choi et al [26] and Calandra et al [27] but not close to the experimentally measured values of Bud’ko et al [4] and Hinks et al [5].

Figure 3 shows the variation of the isotope effect exponent, $\beta$, with the interband electron–plasmon interaction, $\lambda_{\pi\sigma\text{pl}}$ for a set of parameter. We can see that $\beta$ increases with $\lambda_{\pi\sigma\text{pl}}$ but decreases for increasing Coulomb pseudopotential. The variation of $\beta$ with $\lambda_{\pi\sigma}$ for various $\mu^*$ is shown in figure 4. Both the interband contributions of phonon and collective excitations increase with the isotope exponent and tend to saturate at a BCS predicted value of 0.5 for conventional superconductors.

4. Conclusion

We have formulated a two-band model within the Bogoliubov–Valatin [48, 49] formalism and, by incorporating the effect of the collective excitation in the system, we estimated the transition temperature, $T_c \approx 38.80 \text{ K}$ and the isotope effect exponent, $\beta \approx 0.43$. Our analysis shows that the inclusion of electron–phason and electron–plasmon interactions enhances the transition temperature of a superconducting MgB$_2$. Although the model fails to account for the experimentally observed value of $\beta$, it gives evidence that the pairing mechanism in MgB$_2$ is not purely phonon and the effects of interband contributions are not negligible. Thus, more work is needed both theoretically and experimentally to understand the effect of this non-phonon mechanism. This is because only the isotope effect cannot be used to assign the form of the pairing mechanism in a superconducting material and the reduced isotope effect exponent of superconducting MgB$_2$ is still unclear [24].

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