Influence of Interband Interaction on Isotope Effect Exponent of MgB$_2$ Superconductors

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**Abstract**

The exact formula of $T_c$’s equation and the isotope effect exponent of two-band s-wave superconductors in weak-coupling limit are derived by considering the influence of interband interaction. The paring interaction in each band consisted of 2 parts: the electron-phonon interaction and non-electron-phonon interaction are included in our model. The isotope effect exponent of MgB$_2$, $\alpha = 0.3$ with $T_c \approx 40$ K, can be found in the weak coupling regime and interband interaction of electron-phonon interaction show more effect on isotope effect exponent than of non-phonon interaction.
1. Introduction

The isotope effect exponent, $\alpha$, is one of the most interesting properties of superconductors. In the conventional BCS theory $\alpha = 0.5$ for all elements. In high-$T_c$ superconductors, experimenters found that $\alpha$ is smaller than 0.5$^{[1-3]}$. This unusual small value leads to suggestion that the pairing interaction might be predominantly of electronic origin with a possible small phononnic contribution$^{[4]}$. To explain the unusual isotope effect in high-$T_c$ superconductors, many models have been proposed such as the van Hove singularity$^{[5-7]}$, anharmonic phonon$^{[8,9]}$, pairing-breaking effect$^{[10]}$, and pseudogap$^{[11,12]}$.

The discovery of$^{[13]}$ of superconductivity in MgB$_2$ with a high critical temperature, $T_c \approx 39$ K, has attracted a lot of considerable attention. Various experiments$^{[14-21]}$ suggest the existence of multiband in MgB$_2$ superconductors. The gap values $\Delta(k)$ cluster into two groups at low temperature, a small value of $\approx 2.5$ meV and a large value of $\approx 7$ meV. The calculation of the electron structure$^{[22-26]}$ support this conclusion. The Fermi surface consists of four sheets: two three-dimensional sheets from the $\pi$ bonding and antibonding bands $(2p_x)$, and two nearly cylindrical sheets from the two-dimensional $\sigma$ band $(2p_y, z)$$^{[24,27]}$. There is a large difference in the electron-phonon coupling on different Fermi surface sheet and this fact leads to multiband description of superconductivity. The average electron-phonon coupling strength is found to be small values$^{[14-16]}$. Ummarino et al.$^{[28]}$ proposed that MgB$_2$ is the weak coupling two band phononic system where the Coulomb pseudopotential and the interchannel paring mechanism are key terms to interpret the superconductivity state. Garland$^{[29]}$ has shown that Coulomb potential in the $d$-orbitals of transition metal reduce the isotope exponent whereas sp-metals generally shown a nearly full isotope effect. So for sp-metal as MgB$_2$, the Coulomb effect could not be account to explain the reduced of isotope exponent.

Budko et al.$^{[30]}$ and Hinks et al.$^{[31]}$ measured the boron isotope exponent and estimated as $\alpha_B = 0.26 \pm 0.03$ and nearly zero magnesium isotope effect. The boron isotope exponent is closed to that obtained for the YNi$_2$B$_2$C and LuNi$_2$B$_2$C borocarbides$^{[32,33]}$ where theoretical work$^{[34]}$ suggested that the phonons responsible for the superconductivity are high-frequency boron optical modes. This observation is consistent with a phonon-mediated BCS superconducting mechanism that boron phonon modes are playing an important role.

The theory of thermodynamic and transport properties of MgB$_2$ was made in the framework of the two band BCS model$^{[35-43]}$. Zhitomirsky and Dao$^{[44]}$ derive the Ginzburg-Landau functional for two gap superconductors from the microscopic BCS model and then investigate the magnetic properties. The concept of multiband superconductors was first introduced by Suhl$^{[45]}$ and Moskalenke$^{[46]}$ in case of large disparity of the electron-phonon interaction for different Fermi-surface sheets.

The purpose of this paper is to derive the exact formula of $T_c$'s equation and the isotope effect exponent of two-band superconductors in weak-coupling limit by considering the influence of interband interaction. The paring interaction in each band consisted of 2 parts: an attractive electron-phonon interaction and an attractive non-electron-phonon interaction are included in our model.

2. Model and calculation

The properties of MgB$_2$ suggest the two-band s-wave superconductors ($\sigma$-band and $\pi$-band). And in each band, it may have two energy
To recover this fact, we make the assumption that the paring interaction consists of 2 parts: an attractive electron-phonon interaction and an attractive non-electron-phonon interaction in \( \sigma \)-band and \( \pi \)-band, and the \( \sigma - \pi \) scattering of interband pairs. The Hamiltonian of the corresponding system is taken in the form

\[
H = H_{\sigma} + H_{\pi} + H_{\pi \sigma}
\]

(1)

where \( H_{\sigma}, H_{\pi}, \text{and} H_{\pi \sigma} \) are the Hamiltonian of \( \pi \) band, \( \sigma \) band and interband respectively that

\[
H_{\pi} = \sum_{k\sigma} \epsilon_{k\sigma} \pi_{k\sigma}^{+} \pi_{k\sigma} - \sum_{k\ell} V_{\pi \ell} \pi_{k\ell}^{+} \pi_{-k\ell}^{+} \pi_{k\ell} \pi_{-k\ell}^{+}
\]

(2.1)

\[
H_{\pi \sigma} = \sum_{k\ell} V_{\pi \ell} \left( \sigma_{k\ell}^{+} \pi_{-k\ell}^{+} \pi_{k\ell} \pi_{-k\ell}^{+} + \pi_{k\ell}^{+} \pi_{-k\ell}^{+} \pi_{k\ell} \pi_{-k\ell}^{+} \right)
\]

(2.3)

Here we use the standard meaning of parameters and \( V_{\pi \ell}, V_{\pi \ell}, V_{\pi \ell} \) are the attractive interaction potential in \( \sigma \) band and \( \pi \) band, and interband respectively.

By performing a BCS mean field analysis of Eq.(1) and applying standard techniques, we obtain the gap equation as

\[
\Delta_{jk} = -\sum_{\ell} V_{\pi \ell} \frac{\Delta_{\ell j}}{2 \sqrt{\epsilon_{\pi \ell}^{2} + \Delta_{\ell j}^{2}}} \tan \left( \frac{\sqrt{\epsilon_{\pi \ell}^{2} + \Delta_{\ell j}^{2}}}{2T} \right) - \sum_{\ell} V_{\pi \ell} \frac{\Delta_{\ell j}}{2 \sqrt{\epsilon_{\pi \ell}^{2} + \Delta_{\ell j}^{2}}} \tan \left( \frac{\sqrt{\epsilon_{\pi \ell}^{2} + \Delta_{\ell j}^{2}}}{2T} \right)
\]

(3.1)

\[
\Delta_{jk} = -\sum_{\ell} V_{\pi \ell} \frac{\Delta_{\ell j}}{2 \sqrt{\epsilon_{\pi \ell}^{2} + \Delta_{\ell j}^{2}}} \tan \left( \frac{\sqrt{\epsilon_{\pi \ell}^{2} + \Delta_{\ell j}^{2}}}{2T} \right) - \sum_{\ell} V_{\pi \ell} \frac{\Delta_{\ell j}}{2 \sqrt{\epsilon_{\pi \ell}^{2} + \Delta_{\ell j}^{2}}} \tan \left( \frac{\sqrt{\epsilon_{\pi \ell}^{2} + \Delta_{\ell j}^{2}}}{2T} \right)
\]

(3.2)

In each band, the paring interaction consists of 2 parts\([47,48]\) : an attractive electron-phonon interaction \( V_{\pi \ell} \) and an attraction non-electron-phonon interaction \( U_{c}, \omega_{b} \) and \( \omega_{c} \) is the characteristic energy cutoff of the Debye phonon and non-phonon respectively. The interaction potential \( V_{\pi \ell} \) may be written as

\[
V_{\pi \ell} = -V_{\pi \ell}^p - U_{c}^{*} \quad \text{for} \quad 0 < \epsilon < \omega_{b}
\]

\[
= -U_{c}^{*} \quad \text{for} \quad \omega_{b} < \epsilon < \omega_{c} \quad \text{and} \quad i = p, \pi , p \pi
\]

For such as the interaction the superconducting order parameter can be written as

\[
\Delta_{jk} = \Delta_{j} \quad \text{for} \quad 0 < \epsilon < \omega_{b}
\]

\[
= \Delta_{j} \quad \text{for} \quad \omega_{b} < \epsilon < \omega_{c} \quad \text{and} \quad j = p, \pi
\]

3. \( T_{c} \)'s Equation

In this section, the exact formula of \( T_{c} \)'s equation of two- band \( s \)-wave superconductors is derived. At \( T = T_{c} \) and constant density of state \( N(\epsilon) = N(0) \), Eq.(3) become
\[
\begin{pmatrix}
\Delta_{m} \\
\Delta_{p1} \\
\Delta_{\lambda_2} \\
\Delta_{p2}
\end{pmatrix} =
\begin{pmatrix}
(\lambda_{\pi} + \mu_{\pi})I_{1} & (\lambda_{\pi p} + \mu_{\pi p})I_{1} & \mu_{\pi}I_{2} & 0 \\
(\lambda_{\pi} + \mu_{\pi})I_{1} & (\lambda_{\pi p} + \mu_{\pi p})I_{1} & 0 & \mu_{\pi}I_{2} \\
\mu_{\pi}I_{1} & \mu_{\pi}I_{1} & \mu_{\pi}I_{2} & \mu_{\pi}I_{2} \\
\mu_{\pi}I_{1} & \mu_{\pi}I_{1} & \mu_{\pi}I_{2} & \mu_{\pi}I_{2}
\end{pmatrix}
\begin{pmatrix}
\Delta_{x1} \\
\Delta_{p1} \\
\Delta_{x2} \\
\Delta_{p2}
\end{pmatrix}
\] (6)

Here
\[
I_{1} = \int_{0}^{\infty} d\omega \frac{\tanh(\epsilon / 2T_{c})}{\epsilon}
\]

and
\[
I_{2} = \int_{0}^{\infty} d\omega \frac{\tanh(\epsilon / 2T_{c})}{\epsilon}
\]

are the coupling constants.

Solving the secular equation , the appropriate solution is,
\[
I_{1} = \frac{A}{B + \sqrt{C^2 - D}}
\]

that
\[
A = 2(1 + \mu_{p})(-1 + \mu_{\pi}) - 2I_{2}\mu_{p}^{2}
\]
\[
B = \mu_{p} + \mu_{\pi} + 2I_{2}(-\mu_{p}\mu_{\pi} + \mu_{\pi}^{2}) + (\lambda_{\pi} + \lambda_{\pi})((-1 + \mu_{p})(-1 + \mu_{\pi}) - I_{2}\mu_{p}^{2})
\]
\[
C = \lambda_{\pi} + \lambda_{\pi} + \mu_{p} - 2I_{2}\mu_{p} + (\lambda_{\pi} + \lambda_{\pi})(1 + \mu_{p}(\lambda_{\pi} + \lambda_{\pi}) - I_{2}(\lambda_{\pi} + \lambda_{\pi} + 2\mu_{p})
\]
\[
- I_{2}\mu_{p}^{2}(-2 + I_{2}(\lambda_{\pi} + \lambda_{\pi}))
\]
\[
D = 4((-1 + \mu_{p})(-1 + \mu_{\pi}) - I_{2}\mu_{p}^{2})(\lambda_{\pi}\mu_{p} - 2\lambda_{\pi}\mu_{p}) - (1 + I_{2}\lambda_{\pi})(\mu_{p}\mu_{\pi} - \mu_{\pi}^{2})
\]
\[
+ \lambda_{p}(-1 + \mu_{p}(-\mu_{\pi} + \lambda_{\pi}(-1 + \mu_{\pi})) - I_{2}\mu_{p}^{2}(-1 + I_{2}\lambda_{\pi}))
\]
\[
+ \lambda_{\pi}^{2}(-1 + I_{2}(\mu_{p} + \mu_{\pi}) + I_{2}(-\mu_{p}\mu_{\pi} + \mu_{\pi}^{2}))
\]

Eq.(8) is the Tc’s equation of two-band s-wave superconductors.

4. The isotope effect exponent

In harmonic approximation , \(\omega_0 \propto M^{1/2}\), and \(\omega_0\) does not depend on mass.

The isotope effect exponent can be derived from the equation
\[
\alpha = \frac{1}{2} \frac{d \ln T_{c}}{d \ln M}
\]

where M is the mass of the atom constituting the specimen under consideration.

Using Eq.(6) and Eq.(9), we can the isotope effect exponent as below

\[
\alpha = \frac{(1 / 2)}{\tanh(\omega_{0} / 2T_{c})} \frac{\mu_{\pi}D' + \mu_{\pi}E' + \mu_{\pi}^{2}F'}{\tanh((\omega_{0} / 2T_{c}))} \left( \lambda_{\pi}^{2}A' + I_{2}\lambda_{\pi}B' + \lambda_{\pi}^{2}C' \right) - 1
\]

(10)
Here

\[ A' = \{-1 + \mu_p (I_1 + I_2)\}[-1 + \mu_x (I_1 - I_2)] + (I_1^2 - I_2^2)\mu_{xp} \]

\[ B' = \lambda_{xp}[2(-1 + I_2\mu_p)(-1 + I_2\mu_p) + I_1(\mu_p + \mu_x - 2I_2\mu_p\mu_{xp})] + 4\mu_{xp} + 2(I_1 - I_2)I_2\lambda_{xp}\mu_{np}^2 \]

\[ C' = (-1 + I_2\mu_p)(-1 + I_2\mu_p) + I_2^2\mu_{np}^2 + I_1'[\{-\mu_x + \mu_p(-1 + 2I_2\mu_p) - 2I_2\mu_{np}^2\} \]

\[ + I_1\mu_p - \mu_{xp} + 2\mu_{np}(-1 + I_2\mu_p)(-1 + I_2\mu_p) + I_1^2\mu_{np}^2] \]

\[ D' = I_1^2\lambda_{xp}^2 - (-1 + I_1\lambda_{xp})(-1 + I_1\lambda_{xp}) \]

\[ E' = -1 + I_1(\lambda_{xp} + \lambda_{xp}(1 - I_1\lambda_{np}) + I_1\lambda_{np}^2) + \mu_x F \]

\[ F' = 2I_2 + I_1(2 - 2I_2(\lambda_{np} + \lambda_{np}) + I_1(-\lambda_{np} + \lambda_{np})(-1 + 2I_2\lambda_{np}) - 2I_2\lambda_{np}^2) \]

Eq.(8) and Eq.(10) can be easily reduced to the $T_c$’s equation and isotope exponent of BCS theory.

In Figure.(1), we plot a three dimensional graph of the isotope exponent Eq.(10) versus the interband coupling constant $\lambda_{np}$ and $\mu_{np}$. Depending on the measured Debye frequency $\omega_0 = 64.3$ meV [30,49] and $T_c \approx 40$ K, the parameters are $T_c = 40$ K, $\omega_0 = 745$ K, $\omega_c = 1.5\omega_0$, $\lambda_x = \lambda_p = 0.05$, $\mu_x = \mu_p = 0.05$. The isotope effect exponent is tend to 0.5 at large values of phonon and low value of non-phonon interband coupling constant. We calculate Eq.(8) and Eq.(10) numerically to find isotope effect exponent of MgB$_2$, $\alpha = 0.3$ with $T_c \approx 40$ K that many ranges of coupling constant agree with these conditions, example as $\mu_x = \mu_p = 0.05$, $\lambda_{xp} = 0.05$, $\mu_{np} = 0.142$, $0.034 < \lambda_p < 0.114$, and $0.01 < \lambda_x < 0.1$. In Figure.(2), we show the effect of interband coupling constant on isotope effect exponent. The interband interaction of electron-phonon interaction show more effect on isotope exponent than of non-phonon interaction and both of them increase the isotope effect exponent in the same way.

5.Conclusions

The exact formula of $T_c$’s equation and the isotope effect exponent of two-band s-wave superconductors in weak-coupling limit are derived by considering the influence of interband interaction. The paring interaction in each band consisted of 2 parts: an attractive electron-phonon interaction and an attractive non-electron-phonon interaction are included. We find isotope effect exponent of MgB$_2$, $\alpha = 0.3$ with $T_c \approx 40$ K in many ranges of coupling constant. These strength values of the coupling parameters indicate that the MgB$_2$ superconductor is in the weak coupling regime. The interband interaction of electron-phonon interaction show more effect on isotope exponent than of non-phonon interaction.
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Figure Caption

**Figure (1).** Plot graph of the isotope exponent Eq.(10) versus the interband coupling constant $\lambda_{np}$ and $\mu_{np}$, the parameters are $T_c = 40$ K, $\omega_0 = 745$ K, $\omega_c = 1.5\omega_0$, $\lambda_\pi = \lambda_p = 0.05$, $\mu_\pi = \mu_p = 0.05$.

**Figure (2).** We show the effect of interband coupling constant on isotope effect exponent. The parameters are $T_c = 40$ K, $\omega_0 = 745$ K, $\omega_c = 1.5\omega_0$, $\lambda_p = 0.1$, $\mu_\pi = \mu_p = 0.05$.
Figure (1).

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Figure (2).

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