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Effect 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 the weak-coupling limit are derived by considering the influence of interband interaction. In each band, our model consists of two pairing interactions: the electron–phonon interaction and non-electron–phonon interaction. We find that 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 shows more effect on the isotope effect exponent than on the interband interaction of non-phonon.

Keywords. Isotope effect exponent; superconductors; interband interaction.

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1. Introduction

The isotope effect exponent, α, 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, it is found that α is smaller than 0.5 [1–3]. This unusually small value suggests that the pairing interaction might be predominantly of electronic origin with a possibly small phononic 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 superconductivity [13] in MgB_2 with a high critical temperature, $T_c \approx 39$ K, has attracted a lot of attention. Various experiments [14–21] suggest the existence of mutiband in MgB_2 superconductors. The gap values $\Delta(k)$ cluster into two groups at low temperature: a small value of ≈2.5 meV and a large value of ≈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 π bonding and antibonding bands ($2p_z$), and two nearly cylindrical sheets from the two-dimensional σ band ($2p_{x,y}$) [24,27]. There is a large difference in the electron–phonon coupling on different Fermi surface sheets and this leads to multiband description of superconductivity. The average electron–phonon coupling strength is found to have small values [14–16]. Ummarino *et al* [28] proposed that MgB_2 is a weak coupling two-band phononic system where the Coulomb pseudopotential and the interchannel pairing mechanism are key terms to interpret the superconductivity state. Garland [29] has shown that Coulomb potential in the d-orbitals of the transition metal reduced the isotope exponent whereas sp-metals generally show a nearly full isotope effect. Thus, like sp-metal, for MgB_2 the Coulomb effect cannot be taken into account to explain the reduction of the isotope exponent.

Budko *et al* [30] and Hinks *et al* [31] measured the boron isotope exponent and found that $\alpha_B = 0.26 \pm 0.03$ and nearly zero of the magnesium isotope exponent. The boron isotope exponent is close to that obtained for YNi_2B_2C and $LuNi_2B_2C$ borocarbides [32,33] whereas 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 which indicates that boron phonon modes play 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] derived the Ginzburg–Landau functional for the two-gap superconductors from the microscopic BCS model and then investigated the magnetic properties. The concept of multiband superconductors was first introduced by Suhl *et al* [45] and Moskalenko *et al* [46] in case of large disparity of the electron–phonon interaction for different Fermi-surface sheets. Okoye [47] studied the isotope shift exponent of the two-band BCS gap equation that two bands have identical characteristic with a linear energy-dependent electronic density of state, and electron–phonon and negative–U centre interaction mechanisms.

The purpose of this paper is to derive the exact formula of T_c's equation and the isotope effect exponent of the two-band superconductors that two bands have non-identical characteristic in weak-coupling limit by considering the influence of interband interaction. The pairing interaction in each band consists of two parts: an attractive electron–phonon interaction and an attractive non-electron–phonon interaction.

2. Model and calculation

Experiments suggest that MgB_2 is the two-band s-wave superconductor (σ-band and π-band). It may have two energy gaps in each band. To recover this fact, we make the assumption that the pairing interaction consists of two parts: an attractive electron–phonon interaction and an attractive non-electron–phonon interaction in σ-band and π-band, and the σ–π scattering of interband pairs.

The Hamiltonian of the corresponding system is taken as [47]

$$H = H_\pi + H_p + H_{p\pi}, \tag{1}$$

where H_π, H_p and $H_{p\pi}$ are the Hamiltonians of the π-band, the σ-band and the interband respectively.

$$H_\pi = \sum_{k\sigma} \varepsilon_{\pi k\sigma} \pi^+_{k\sigma} \pi_{k\sigma} + \sum_{kk'} V_{\pi\pi kk'} \pi^+_{k\uparrow} \pi^+_{-k\downarrow} \pi_{-k'\downarrow} \pi_{k'\uparrow}, \tag{2a}$$

$$H_p = \sum_{k\sigma} \varepsilon_{pk\sigma} p^+_{k\sigma} p_{k\sigma} + \sum_{kk'} V_{ppkk'} p^+_{k\uparrow} p^+_{-k\downarrow} p_{-k'\downarrow} p_{k'\uparrow}, \tag{2b}$$

$$H_{p\pi} = \sum_{kk'} V_{p\pi kk'} (p^+_{k\uparrow} p^+_{-k\downarrow} \pi_{-k'\downarrow} \pi_{k'\uparrow} + \pi^+_{k\uparrow} \pi^+_{-k\downarrow} p_{-k'\downarrow} p_{k'\uparrow}). \tag{2c}$$

Here we use the standard meaning of parameters and $\sum_{k\sigma}$ represents the summation over wave vector $\vec{k}$ and spin σ. $V_{\pi\pi kk'}$, $V_{ppkk'}$, $V_{p\pi kk'}$ are the attractive interaction potentials in the σ-band, the π-band and the interband respectively.

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

$$\Delta_{pk} = -\sum_{k'} V_{ppkk'} \frac{\Delta_{pk'}}{2\sqrt{\varepsilon^2_{pk'} + \Delta^2_{pk'}}} \tanh\left(\frac{\sqrt{\varepsilon^2_{pk'} + \Delta^2_{pk'}}}{2T}\right) - \sum_{k'} V_{p\pi kk'} \frac{\Delta_{\pi k'}}{2\sqrt{\varepsilon^2_{\pi k'} + \Delta^2_{\pi k'}}} \tanh\left(\frac{\sqrt{\varepsilon^2_{\pi k'} + \Delta^2_{\pi k'}}}{2T}\right), \tag{3a}$$

$$\Delta_{\pi k} = -\sum_{k'} V_{\pi\pi kk'} \frac{\Delta_{\pi k'}}{2\sqrt{\varepsilon^2_{\pi k'} + \Delta^2_{\pi k'}}} \tanh\left(\frac{\sqrt{\varepsilon^2_{\pi k'} + \Delta^2_{\pi k'}}}{2T}\right) - \sum_{k'} V_{p\pi kk'} \frac{\Delta_{pk'}}{2\sqrt{\varepsilon^2_{pk'} + \Delta^2_{pk'}}} \tanh\left(\frac{\sqrt{\varepsilon^2_{pk'} + \Delta^2_{pk'}}}{2T}\right). \tag{3b}$$

In each band, the pairing interaction consists of two parts [48,49]: an attractive electron–phonon interaction V_{ph} and an attractive non-electron–phonon interaction $U_{\rm c}$. $\omega_{\rm D}$ and $\omega_{\rm c}$ are the characteristic energy cut-off of the Debye phonon and non-phonon respectively. The non-electron–phonon interaction may be the exchange of attractive free-carrier negative-U centre interaction.

The interaction potential $V_{kk'}$ may be written as

$$V_{ikk'} = -V^i_{ph} - U^i_{\rm c}, \tag{4a}$$

for $0 < |\varepsilon_k| < \omega_{\rm D}$ and $0 < |\varepsilon_{k'}| < \omega_{\rm D}$ and

$$V_{ikk'} = -U^i_{\rm c} \tag{4b}$$

for $\omega_{\rm D} < |\varepsilon_k| < \omega_{\rm c}$ and $\omega_{\rm D} < |\varepsilon_{k'}| < \omega_{\rm c}$, where $i = p, \pi, p\pi$.

For such interactions, the superconducting order parameters can be written as

$$\begin{aligned} \Delta_{jk} &= \Delta_{j1}, \quad \text{for } 0 < |\varepsilon| < \omega_{\rm D}, \\ &= \Delta_{j2}, \quad \text{for } \omega_{\rm D} < |\varepsilon| < \omega_{\rm c} \text{ and } j = p, \pi. \end{aligned} \tag{5}$$

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 $N(\varepsilon_k) = N(0)$, eq. (3) becomes

$$\begin{pmatrix} \Delta_{\pi 1} \\ \Delta_{p1} \\ \Delta_{\pi 2} \\ \Delta_{p2} \end{pmatrix} = \begin{pmatrix} (\lambda_\pi + \mu_\pi)I_1 & (\lambda_{\pi p} + \mu_{\pi p})I_1 & \mu_\pi I_2 & \mu_{\pi p} I_2 \\ (\lambda_{\pi p} + \mu_{\pi p})I_1 & (\lambda_p + \mu_p)I_1 & \mu_{\pi p} I_2 & \mu_p I_2 \\ \mu_\pi I_1 & \mu_{\pi p} I_1 & \mu_\pi I_2 & \mu_{\pi p} I_2 \\ \mu_{\pi p} I_1 & \mu_p I_1 & \mu_{\pi p} I_2 & \mu_p I_2 \end{pmatrix} \begin{pmatrix} \Delta_{\pi 1} \\ \Delta_{p1} \\ \Delta_{\pi 2} \\ \Delta_{p2} \end{pmatrix}. \tag{6}$$

Here

$$I_1 = \int_0^{\omega_D} \mathrm{d}\varepsilon \frac{\tanh(\varepsilon/2T_c)}{\varepsilon}, \tag{7a}$$

$$I_2 = \int_{\omega_D}^{\omega_c} \mathrm{d}\varepsilon \frac{\tanh(\varepsilon/2T_c)}{\varepsilon} \tag{7b}$$

and

$$\lambda_\pi = N_\pi(0)V_{ph}^\pi, \quad \lambda_p = N_p(0)V_{ph}^p, \quad \lambda_{\pi p} = N_\pi(0)V_{ph}^{\pi p} = N_p(0)V_{ph}^{p\pi},$$
$$\mu_\pi = N_\pi(0)U_c^\pi, \quad \mu_p = N_p(0)U_c^p, \quad \mu_{\pi p} = N_\pi(0)U_c^{\pi p} = N_p(0)U_c^{p\pi}.$$

Here λ and μ are the coupling constants of phonon and non-phonon respectively. Solving the secular equation, we get

$$I_1 = \frac{A}{B + \sqrt{C^2 - D}}, \tag{8}$$

where

$$\begin{aligned} A &= 2(-1 + I_2\mu_p)(-1 + I_2\mu_\pi) - 2I_2^2\mu_{\pi p}^2, \\ B &= \mu_p + \mu_\pi + 2I_2(-\mu_p\mu_\pi + \mu_{\pi p}^2) + (\lambda_p + \lambda_\pi) \\ &\quad \times((-1 + I_2\mu_p)(-1 + I_2\mu_\pi) - I_2^2\mu_{\pi p}^2)), \\ C &= \lambda_p + \lambda_\pi + \mu_p - I_2\mu_p(\lambda_p + \lambda_\pi) + \mu_\pi(1 + I_2^2\mu_p(\lambda_p + \lambda_\pi) \\ &\quad -I_2(\lambda_p + \lambda_\pi + 2\mu_p)) - I_2\mu_{\pi p}^2(-2 + I_2(\lambda_p + \lambda_\pi)), \\ D &= 4((-1 + I_2\mu_p)(-1 + I_2\mu_\pi) - I_2^2\mu_{\pi p}^2) \\ &\quad \times[\lambda_\pi\mu_p - 2\lambda_{\pi p}\mu_{\pi p} - (-1 + I_2\lambda_\pi)(\mu_p\mu_\pi - \mu_{\pi p}^2) \\ &\quad +\lambda_p[(-1 + I_2\mu_p)(-\mu_\pi + \lambda_\pi(-1 + I_2\mu_\pi)) - I_2\mu_{\pi p}^2(-1 + I_2\lambda_\pi)] \\ &\quad +\lambda_{\pi p}^2(-1 + I_2(\mu_p + \mu_\pi) + I_2^2(-\mu_p\mu_\pi + \mu_{\pi p}^2))]. \end{aligned}$$

Equation (8) is the T_c's equation of the two-band s-wave superconductors that can be reduced to a one-band superconductor with non-phonon interaction by taking $\Delta_2 = 0$. It can also be a two-band superconductor without non-phonon interaction by taking $\mu = 0$ that agree with the T_c's equation of Ketterson and Song [50].

4. The isotope effect exponent

In the harmonic approximation, $\omega_{\rm D}\alpha M^{-1/2}$, and $\omega_{\rm c}$ does not depend on mass. The isotope effect exponent can be derived from the equation

$$\alpha = -\frac{{\rm d}\ln T_{\rm c}}{{\rm d}\ln M} = \frac{1}{2}\frac{\omega_{\rm D}}{T_{\rm c}}\frac{{\rm d}T_{\rm c}}{{\rm d}\omega_{\rm D}}, \tag{9}$$

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

Using eqs (6) and (9), we can find the isotope effect exponent to be

$$\alpha = \frac{(1/2)}{\frac{\tanh(\omega_{\rm c}/2T_{\rm c})}{\tanh((\omega_{\rm D}/2T_{\rm c}))}\frac{(\mu_\pi D'+\mu_p E'+\mu_{\pi p}^2 F')}{(\lambda_\pi A'+I_1\lambda_{\pi p}B'+\lambda_p C')} - 1}. \tag{10}$$

Here

$$\begin{aligned}
A' &= -[-1+\mu_p(I_1+I_2)][-1+\mu_\pi(I_1-I_2)] + (I_1^2-I_2^2)\mu_{\pi p}^2,\\
B' &= \lambda_{\pi p}[2(-1+I_2\mu_p)(-1+I_2\mu_p) + I_1(\mu_p+\mu_\pi-2I_2\mu_p\mu_\pi)]\\
&\quad +4\mu_{\pi p} + 2(I_1-I_2)I_2\lambda_{\pi p}\mu_{\pi p}^2,\\
C' &= (-1+I_2\mu_p)(-1+I_2\mu_\pi) + I_2^2\mu_{\pi p}^2\\
&\quad +I_1^2[-\mu_\pi+\mu_p(-1+2I_2\mu_\pi)-2I_2\mu_{\pi p}^2]\\
&\quad +I_1[\mu_p-\mu_\pi+2\lambda_\pi(-(-1+I_2\mu_p)(-1+I_2\mu_\pi)+I_2^2\mu_{\pi p}^2)],\\
D' &= I_1^2\lambda_{\pi p}^2 - (-1+I_1\lambda_p)(-1+I_1\lambda_\pi),\\
E' &= -1+I_1(\lambda_\pi+\lambda_p(1-I_1\lambda_\pi)+I_1\lambda_{\pi p}^2)+\mu_\pi F,\\
F' &= 2I_2 + I_1(2-2I_2(\lambda_p+\lambda_\pi)\\
&\quad +I_1(-\lambda_\pi+\lambda_p(-1+2I_2\lambda_\pi)-2I_2\lambda_{\pi p}^2).
\end{aligned}$$

Equation (10) can be easily reduced to be the isotope effect exponent of the BCS theory.

We calculate eqs (8) and (10) numerically to find the isotope effect exponent of MgB_2, $\alpha = 0.3$ with $T_{\rm c} \approx 40$ K and measured Debye frequency $\omega_{\rm D} = 64.3$ meV [30,51]. In figure 1, we show a three-dimensional graph of the isotope exponent (eq. (10)) versus the interband coupling constant $\lambda_{\pi p}$ and $\mu_{\pi p}$. The parameters are $T_{\rm c} = 40$ K, $\omega_{\rm D} = 745$ K, $\omega_{\rm c} = 1.5\omega_{\rm D}$, $\lambda_\pi = \lambda_p = 0.05$ and $\mu_\pi = \mu_p = 0.05$. The value of the isotope effect exponent tend to 0.5 at large values of phonon and low value of non-phonon interband coupling constant. We find that many ranges of coupling constant agree with above conditions, e.g. $\mu_\pi = \mu_p = 0.05$, $\lambda_{\pi p} = 0.05$, $\mu_{\pi p} = 0.142$, $0.034 < \lambda_p < 0.114$, and $0.01 < \lambda_\pi < 0.1$. In figure 2, we show the effect of the interband coupling constant on the isotope effect exponent. The interband interaction of the electron–phonon interaction shows more effect on the isotope exponent than the non-phonon interaction and both of them increase the isotope effect exponent in the same way. The strength of the coupling constant (λ, μ) that we use are in weak-coupling limit that agree with Golubov and Mazin [52]. They considered the weakly coupled superconductor with the impurity of the multiband superconductor and the strength of the coupling constant can be increased to the range of Choi *et al* [53] that an average electron–phonon coupling constant equal to 0.61.

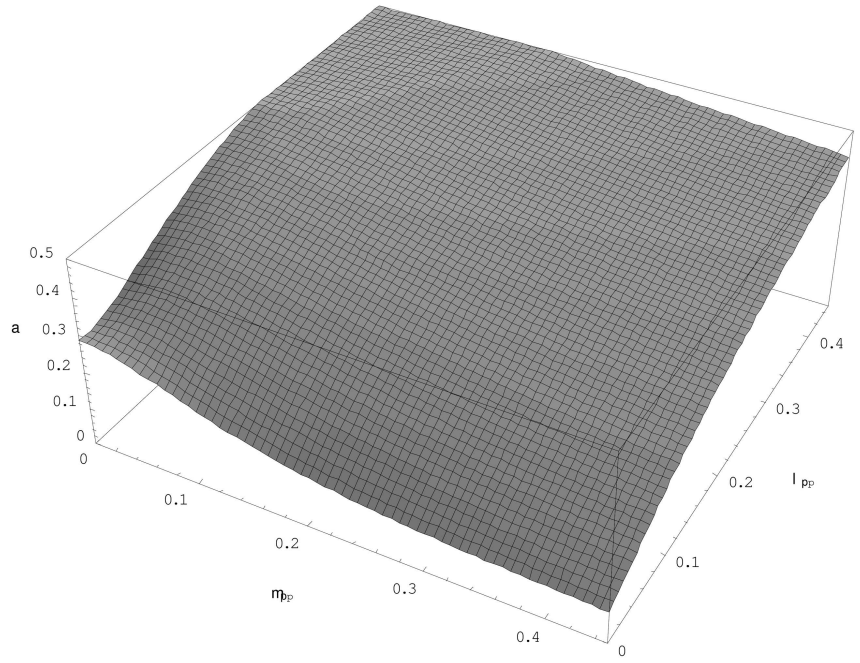

Figure 1. Plot of the isotope exponent (eq. (10)) vs. the interband coupling constant $\lambda_{\pi p}$ and $\mu_{\pi p}$. The parameters are $T_c = 40$ K, $\omega_D = 745$ K, $\omega_c = 1.5\omega_D$, $\lambda_\pi = \lambda_p = 0.05$, $\mu_\pi = \mu_p = 0.05$.

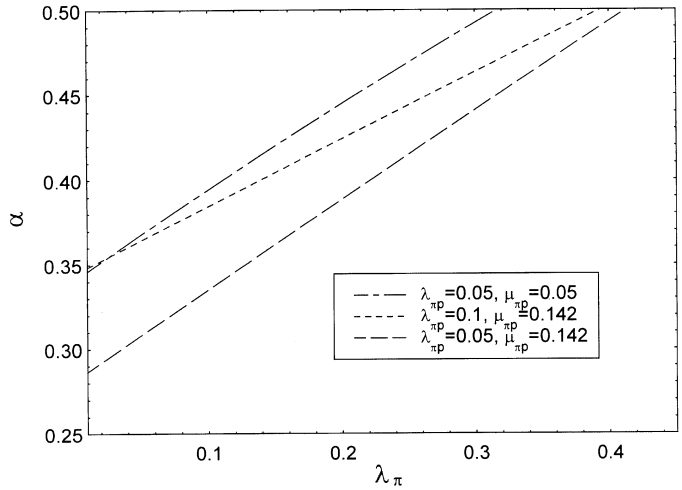

Figure 2. Effect of the interband coupling constant on the isotope effect exponent. The parameters are $T_c = 40$ K, $\omega_D = 745$ K, $\omega_c = 1.5\omega_D$, $\lambda_p = 0.1$, $\mu_\pi = \mu_p = 0.05$.

5. Conclusions

The exact formula of T_c's equation and the isotope effect exponent of the two-band s-wave superconductors in weak-coupling limit are derived by considering the influence of interband interaction. The pairing interaction in each band consists of two parts: an attractive electron–phonon interaction and an attractive non-electron–phonon interaction. We find isotope effect exponent of MgB_2, $\alpha = 0.3$ with $T_c \approx 40$ K in many ranges of coupling constant in the weakly coupling limit. The non-phonon interaction is an important factor that reduced the other into weakly coupling limit. Within our calculation, the strength of the coupling parameters indicate that the MgB_2 superconductor is in the weak coupling regime. The interband interaction of the electron–phonon interaction shows more effect on the isotope exponent than on the non-phonon interaction.

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