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Isotope and interband effects in a multi-band model of superconductivity

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Abstract. Isotope effects (IEs) are essential in determining the pairing mechanism in superconductors. Whereas for Bardeen–Cooper–Schrieffer (BCS)-type superconductors, a clear consensus about IE exists, this is unknown in multiband superconductors (MBSs). We demonstrate here that for MBSs the IEs on the superconducting transition temperature can vary between the BCS value and zero as long as the intraband couplings are affected. It can, however, exceed the BCS value when interband effects are dominant. In both cases, a sign reversal is excluded. In addition, we show that interband coupling contributes substantially to enhancement of T_c. The results are independent of the pairing symmetry and the system-specific band structure. Specifically, we do not address the IEs originating from the MBSs with respect to a specific superconductor, but rather study its emergence within this model and explore all possible sources within the weak coupling theory.

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Multiband superconductivity (MBS) was proposed to be realized in more complex rather than elemental superconductors shortly after the Bardeen–Cooper–Schrieffer (BCS) theory was introduced [1, 2]. Subsequently, the model was theoretically studied in detail [3, 4], but then ignored for a long time because of the lack of experimental realization. Only in 1980 was MBS observed in Nb-doped $SrTiO_3$ [5], but without receiving much attention, possibly because of the very low superconducting transition temperature. After the discovery of high-temperature superconductivity in copper oxides [6], various experiments implicitly suggested the existence of two or more superconducting energy gaps [7–10]. An account of this scenario was given subsequently [11], by interpreting various experimental inconsistencies as originating from two superconducting gaps with different order parameters, namely s + d. It should be mentioned here that s + d symmetry does not necessarily require the existence of two gaps with different symmetries, but could also originate from orthorhombic or tetragonal lattice distortions, as discussed in [12]. Recently, however, a variety of data obtained from μSR techniques have clearly supported the idea of the existence of two gaps and have evidenced that s + d wave superconductivity could be generic to copper oxides [13–16]. In view of the large class of copper oxide superconductors, more experiments are, however, needed. With the discovery of MBS in MgB_2 [17], efforts to observe this unusual phenomenon in other superconductors have increased. MBS was not observed in many metals for many years because it occurs in the 'clean limit' [18] where the single-electron interband inelastic scattering is suppressed. In fact, in the standard BCS approximation a single large Fermi surface is considered since the metal is assumed to be in the dirty limit where the single-electron interband inelastic scattering reduces a multiband system to a single effective band. The clean limit was considered to be impossible because of the presence of impurities or dislocations. However, it was proposed to be possible when the bands have different symmetry, which does not admit single-electron transfer between bands but allows the possibility for pair transfer in the superconducting interband pairing [19]. This point has been proved in doped MgB_2 where MBS driven by interband pairing also remains active in heavily doped samples [20].

After MgB_2 various superconductors have been shown to be two-gap or MBSs superconductors (for a review, see [18]). The newly discovered Fe-based superconductors [21] are undoubtedly MBSs no matter which structural family they belong to. Here, the coupled superconducting order parameters have been suggested to be +/−s-wave [22] as it is well known in the case when the interband coupling is driven by repulsive Coulomb interaction [18].

An interesting discussion on the origin of superconductivity in the latter material class emerged only very recently, when it became possible to measure isotope effects (IE) on T_c for various classes of these compounds [23–26]. Unfortunately, the data do not permit us to draw conclusions, since for one and the same compound different experimental groups report controversial results, namely a conventional [20, 23] and a sign-reversed [24, 25] isotope effect exponent (IEE) on T_c.

Theoretically, little effort has been made to derive the IE within the MBS model, and in the few existing approaches [27, 28] some rather crude approximations have been introduced that seriously and unphysically affect the results [29].

Here, we do not address the IE originating from the MBS model with respect to a specific superconductor, but instead study its emergence within this model and explore all of its possible sources within the weak coupling theory. The latter is justified by the fact that all involved coupling constants are small, i.e. <0.5. From this analysis, we conclude that this model does not admit a sign-reversed isotope effect, whereas a zero effect is possible. This finding is

independent of the symmetry of the coupled order parameters and *independent* of the system's band structure. Also, we address a feature that is typical of this model, namely the T_c-enhancing effect resulting from interband interactions [27, 28]. This can lead to rather exotic isotope effects, which could be realized in systems with unconventional pairing interactions.

The MBS model has been studied in detail in the past and in recent years [1–4, 30–32]. The Hamiltonian is

$$H = \sum_{n,k,\sigma} \varepsilon_n(k) c^+_{n,k\sigma} c_{n,k\sigma} - \sum_{k,k'} V_{ii}(k,k') c^+_{i,k\uparrow} c^+_{i,-k\downarrow} c_{i,-k'\downarrow} c_{i,k'\uparrow} - \sum_{k,k'} V_{jj}(k,k') c^+_{j,k\uparrow} c^+_{j,-k\downarrow} c_{j,-k'\downarrow} c_{j,k'\uparrow} - \sum_{k,k'} V_{ij}(k,k') c^+_{i,k\uparrow} c^+_{i,-k\downarrow} c_{j,-k'\downarrow} c_{j,k'\uparrow} - \sum_{k,k'} V_{ji}(k,k') c^+_{j,k\uparrow} c^+_{j,-k\downarrow} c_{i,-k'\downarrow} c_{i,k'\uparrow}. \quad (1)$$

Here, ε_n $(n = i, j)$ are the momentum(k)-dependent band energies of bands $n = i, j$ considered, with electron creation and annihilation operators c^+ and c and spin index σ. The attractive intraband pairing interactions are denoted by V_{ii}, whereas the interband coupling terms are given by V_{ij}. Note that these pairing terms are either due to a BCS-type electron–phonon attractive potential or due to an unspecified non-phononic mechanism. Its explicit form is not relevant to the results. The coupled gap equations can be derived in the usual way [24, 26] from the above Hamiltonian and are explicitly given by

$$H_i = -\sum_{k'_i} [\Delta_{k'_i} c^+_{k'_i\uparrow} c^+_{-k_i\downarrow} + \Delta^*_{k'_i} c_{-k'_i\downarrow} c_{k_i\uparrow}] + \sum_{k_i,k'_i} V_{ii}(k_i,k'_i) \left\langle c^+_{k_i\uparrow} c^+_{-k_i\downarrow} \right\rangle \left\langle c_{-k'_i\downarrow} c_{k'_i\uparrow} \right\rangle \quad (2a)$$

$$H_{ij} = -\sum_{k_i,k_j} [V_{ij}(k_i,k_j) \langle c^+_{i,k_i\uparrow} c^+_{-i,k_i\downarrow} \rangle c_{j,-k_j\downarrow} c_{j,k_j\uparrow} + V_{ij}(k_i,k_j) \langle c_{j,-k_j\downarrow} c_{j,k_j\uparrow} \rangle c^+_{i,k_i\uparrow} c^+_{i,-k_i\downarrow} + V^*_{ij}(k_i,k_j) c^+_{j,k_j\uparrow} c^+_{j,-k_j\downarrow} \langle c_{i,-k_i\downarrow} c_{i,k_i\uparrow} \rangle + V^*_{ij}(k_i,k_j) c_{i,-k_i\downarrow} c_{i,k_i\uparrow} \langle c^+_{j,k_j\uparrow} c^+_{j,-k_j\downarrow} \rangle - V_{ij}(k_i,k_j) \langle c^+_{i,k_i\uparrow} c^+_{i,-k_i\downarrow} \rangle \langle c_{j,-k_j\downarrow} c_{j,k_j\uparrow} \rangle - V^*_{ij}(k_i,k_j) \langle c_{i,-k_i\downarrow} c_{i,k_i\uparrow} \rangle \langle c^+_{j,k_j\uparrow} c^+_{j,-k_j\downarrow} \rangle]. \quad (2b)$$

Using the following definitions:

$$\Delta^*_{k'_i} = \sum_{k_i} V_{ii}(k_i,k'_i) \left\langle c^+_{k_i\uparrow} c^+_{-k_i\downarrow} \right\rangle,$$

together with

$$A^*_{k'_i} = \sum_{k_i} V_{ij}(k_i,k'_i) \left\langle c^+_{i,k_i\uparrow} c^+_{i,-k_i\downarrow} \right\rangle,$$

$$B^*_{k'_i} = \sum_{k_j,k'_i} V_{ij}(k_i,k'_i) \langle c^+_{j,k_j\uparrow} c^+_{j,-k_j\downarrow} \rangle, \qquad V^*_{ij} = V_{ij},$$

and applying standard techniques, we arrive at

$$\left\langle c^+_{i,k_i\uparrow} c^+_{i,-k_i\downarrow} \right\rangle = \frac{\bar{\Delta}^*_{k_i}}{2E_{k_i}} \tanh \frac{E_{k_i}}{2k_B T} = \bar{\Delta}^*_{k_i} \Phi_{k_i}, \quad (3a)$$

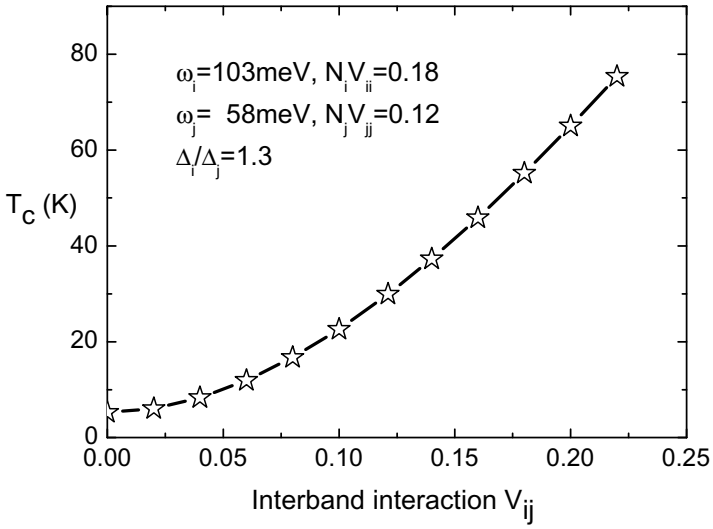

Figure 1. T_c as a function of the interband coupling V_{ij} and fixed intraband interaction energies as given in the figure. N_i, N_j refer to the density of states in the respective band. These values are used throughout. The meaning of the latter is given in the text.

$$\langle c^+_{j,k_j\uparrow} c^+_{j,-k_j\downarrow}\rangle = \frac{\bar{\Delta}^*_{k_j}}{2E_{k_j}} \tanh\frac{E_{k_j}}{2k_BT} = \bar{\Delta}^*_{k_j}\Phi_{k_j} \tag{3b}$$

with $E^2_{k_i} = \varepsilon^2_{k_i} + |\bar{\Delta}_{k_i}|^2$, $\bar{\Delta}_{k_i} = \Delta_{k_i} + A_{k_i}$ and $E^2_{k_j} = \varepsilon^2_{k_j} + |\bar{\Delta}_{k_j}|^2$, $\bar{\Delta}_{k_j} = \Delta_{k_j} + B_{k_j}$. T_c and the superconducting gaps are obtained from the coupled gap equations:

$$\bar{\Delta}_{k_i} = \sum_{k'_i} V_i(k_i, k'_i)\bar{\Delta}_{k'_i}\Phi_{k'_i} + \sum_{k_2} V_{i,j}(k_i, k_j)\bar{\Delta}_{k_j}\Phi_{k_j}, \tag{4a}$$

$$\bar{\Delta}_{k_j} = \sum_{k'_j} V_j(k_j, k'_j)\bar{\Delta}_{k'_j}\Phi_{k'_j} + \sum_{k_1} V_{i,j}(k_i, k_j)\bar{\Delta}_{k_i}\Phi_{k_i}, \tag{4b}$$

which have to be solved self-consistently for each temperature T. T_c is defined by the condition that both gaps become zero simultaneously. The symmetry of the order parameters is contained in the interactions; however, at T_c these are irrelevant.

In the original MBS model as introduced in [1–4], the attractive interactions are considered to arise from electron–phonon interactions. More recently, it was suggested that in a two-band model one band might exhibit a pairing instability arising from antiferromagnetic fluctuations, whereas the other band exhibits electron–phonon-mediated pairing [24, 25]. In such a case, only one channel of this two-component approach can give rise to any isotope effects, whereas the second channel has a zero isotope exponent.

In the following, we restrict the analysis to the two-band case which can be easily extended to the MB case. The two interband pairing interactions are set as equal for transparency, i.e. $V_{ij} = V_{ji}$. Before discussing IEs on T_c, it is essential to demonstrate the effect of the interband interactions on T_c [27, 28]. The results are shown in figure 1, where T_c is shown as a function of the interband coupling. Note that we have chosen the intraband attractive couplings (V_{ii}, V_{jj})

using a constant density of states N_i, N_j to be very distinct from each other in order to obtain gap solutions with different energies. The summations in equations (4) have been replaced by integrals with cutoff energies ω_i, ω_j, as indicated in the figures. Without loss of generality, a zero-temperature gap anisotropy $\Delta_i/\Delta_j = 1.3$ is assumed, which is, e.g., realized in Al-doped MgB_2 [20] and some Fe-based superconductors [21]. Without any anisotropy, isotope effects from either of the channels would be the same.

As can be clearly seen from figure 1, a huge T_c enhancement effect results from the interband coupling *even in the weak coupling analysis*. By raising the interband coupling from zero to 0.2, an increase in T_c by 60 K is obtained. Thus, it is not surprising that two-band superconductors exhibit the high transition temperatures observed in MgB_2, copper oxides and Fe-based compounds. A similar observation has already been made in [3], but, under the assumption that one intraband interaction is repulsive. Also, no quantitative estimates of the T_c enhancement effect have been given in [3], whereas in the present approach (see figure 1) for $V_{ij} = 0$ the T_c value is 5 K, stemming from the larger gap, whereas superconductivity is absent in the second band, and the enhancements with increasing V_{ij} are explicitly given.

The IE on T_c is calculated by assuming that the pairing channel with a larger or a smaller gap stems from electron–phonon interactions, whereas the pairing in the other channel can be due to any other non-phononic mechanism. Also, we have assumed that only those ions contribute to any isotope effect that, e.g., in a multinary compound, are located in the active layers of the superconductor under discussion, namely the CuO_2 layers in copper oxides or the Fe-containing layers in Fe-based superconductors. The calculation of the IEE can explicitly be carried out by considering the cut-off energies to represent either phonon energies that vary with the square root of the inverse ionic mass or any other energy that is independent of this mass. For both situations, the resulting IEE $\alpha = -\mathrm{d}\ln T_c/\mathrm{d}\ln M$(with M being the ionic mass involved) is shown in figure 2, where the changes in T_c are obtained through the same variations in the interband coupling shown in figure 1.

Interestingly, the two IEEs, originating from either the large or the small gap channel alone, depend quite differently on T_c. While the one related to the larger gap decreases from an almost BCS value of $\alpha = 0.5$ for small T_cs to a value around 0.3, the one related to the small gap increases with increasing T_c and converges to the same value for high T_cs as the large gap value. This can be easily understood. For small T_cs the small gap channel loses its weight and does not contribute further, especially when the interband coupling tends to zero. In this case, T_c is given by the closing of the larger gap, and the IEE consequently approaches 0.5. It is also obvious from figure 2 that the IEE always stays positive and can be vanishingly small when only the smaller gap arises from the electron–phonon interaction. An interesting novel and unconventional IEE is obtained under the assumption that the two pairing channels are dominated by non-phononic mechanisms, whereas the interband pairing results from phonon exchange. In this scenario (the inset to figure 2), α rapidly increases with T_c to a maximum value of $\alpha = 0.78$ for $T_c \approx 50$ K to then slightly decrease with further increasing T_c. Even though this picture seems rather unlikely to be realized in existing systems, it is worth observing that the BCS value is not the limit in a phonon-mediated superconductor with both individual components mediated by any other mechanism. In the case when both pairing channels are phonon mediated, α is independent of T_c and adopts the BCS value. The results presented in figure 2 can provide an explanation of the reduced IEE $\alpha = 0.3$ [18] well below the BCS-expected value 0.5 in MgB_2 that remains unexplained [34].

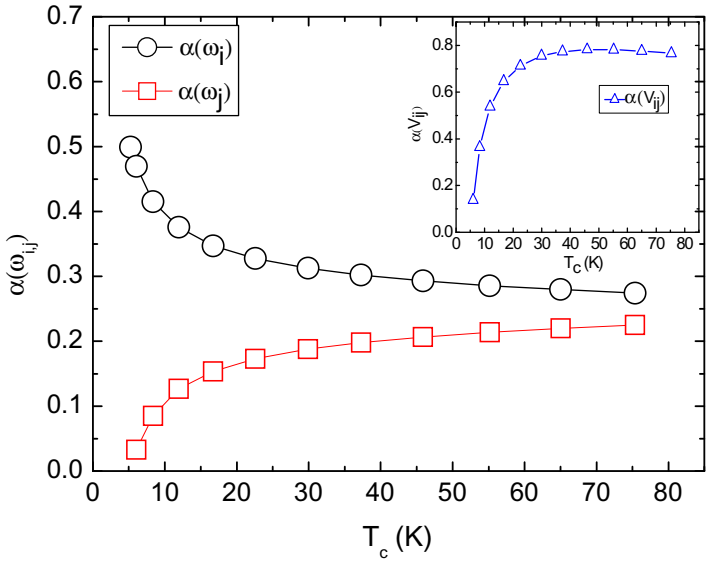

Figure 2. The IEE α as a function of T_c. The open circles refer to the IEE stemming from the larger gap channel being phonon mediated and the smaller one originating from any other pairing interaction, whereas the open squares refer to the reverse situation. The inset to the figure shows the dependence of α on T_c if only the interband interaction is due to electron–phonon interactions.

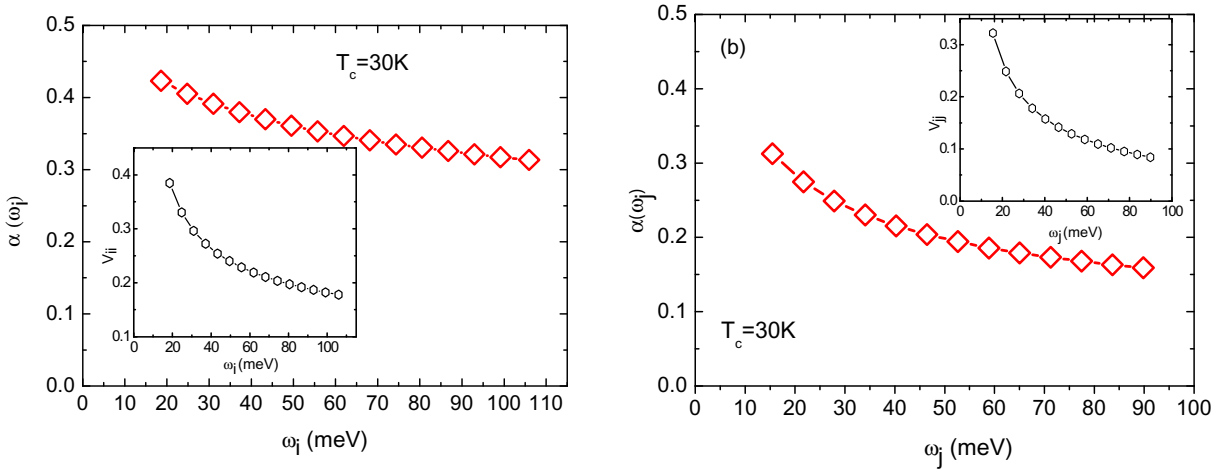

Figure 3. (a) The IEE α as a function of the energy range ω_i related to the larger gap. The inset shows the self-consistent variation of the corresponding intraband interaction. (b) The same as (a), but varying the energy range within the smaller gap channel.

Above we have limited the numerical analysis to the isotope effect as a function of T_c. In the following we consider the case when T_c is fixed ($T_c = 30$ K) and the energy ranges are varied. This requires within Eliashberg theory that the intraband interactions V_{ii} are varied self-consistently in order to keep T_c constant. First we change the energy range ω_i related to the larger gap, as shown in figure 3(a).

The self-consistently obtained variation in the respective intraband coupling is given in the inset to the figure (all other parameters are kept constant). The IEE displays rather large values, ranging from almost 0.45 to 0.3 over the whole energy regime. It increases smoothly with decreasing ω_i and converges to a value around 0.3 for large ω_i. This can be understood by the fact that the intraband coupling V_{ii} rapidly decreases with increasing ω_i and thus loses weight with respect to the second channel. In the alternative case that the energy range ω_j (figure 3(b)) in the smaller gap channel is varied, the IEE shows a similar dependence to that in the previous case, but being substantially reduced (0.35–0.15). Here, the maximum value lies around 0.3 for small ω_j, and decreases to values almost half of that observed for the large gap channel. In both cases the BCS value seems to be out of reach with α always being depressed from it, unless T_c is so small that only the larger gap becomes relevant.

The above analysis of the MBS model should help us to clarify experimental observations of IEs arising in MBS. Our numerical investigation is restricted here to the case when the lattice is harmonic and polaronic effects are absent. Anharmonicity is known to change the IE considerably, and even admits a sign reversal [30], which could offer an explanation of the observed sign-reversed IE of [24, 25]. This case, however, has not been investigated for the MBS model. Obviously, a rather small value of α suggests that the main phononic pairing interaction can be related to the smaller gap channel, whereas values approaching the BCS limit must stem from the channel with the larger gap. Unusually large values, namely $\alpha > 0.5$, must have an unconventional origin, e.g. of polaronic nature: these change the above physics completely. A detailed account of polaronic couplings has already been presented [30, 33, 35–37] and further studies are described elsewhere. However, it is important to note that for a polaronic superconductor the IE depends strongly on the polaronic coupling, which in turn is material dependent. For this reason, we do not address the details here, since the present approach discusses IEs in the general context of MBS.

In summary, we have derived the IE within the weak coupling MBS model and shown that this can approach zero, but never changes sign. The model has been solved rigorously without unphysical assumptions on the energy ranges or the inter- and intra-band interactions, and the results are independent of the pairing symmetries and the system-specific band structure. Even a pronounced momentum-dependent pairing interaction does not change these conclusions since the pairing interaction by definition has to be attractive. In addition to providing insight into possible sources of an IE on T_c, we have also shown that MBS naturally leads to substantially enhanced T_c values as compared to a single-band superconductor. An enhanced IE is expected for a rather exotic pairing mechanism, where the intraband pairing interactions have a non-phononic origin, whereas the interband pairing is caused by the electron–lattice interaction. Within this exhaustive analysis, the observation of an inverse IEE is not possible.

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