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Enhancements of the superconducting transition temperature within the two-band model

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Abstract. The two-band model as introduced by Suhl, Matthias and Walker [Phys. Rev. Lett. **3**, 552 (1959)] accounts for multiple energy bands in the vicinity of the Fermi energy which could contribute to electron pairing in superconducting systems. Here, extensions of this model are investigated wherein the effects of coupled superconducting order parameters with different symmetries and the presence of strong electron-lattice coupling on the superconducting transition temperature T_c are studied. Substantial enhancements of T_c are obtained from both effects.

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Shortly after the BCS theory [1] for superconductivity was presented, Suhl, Matthias and Walker proposed extensions of this theory [2] to account for more complex electronic band structures. Their assumption that pairing might occur in various energy bands that are located in the vicinity of the Fermi energy implied that interband interactions between those bands take place in order to assure a homogeneous superconducting state. Interestingly they observed that a two-order parameter scenario leads to an enhancement of the superconducting transition temperature as compared to a single band model. The two-band model has since then been explored more deeply by various groups [3–6] and has also been invoked recently to explain high temperature superconductivity in copper oxides [7–12] and MgB_2 [13–15]. In this paper we study new extensions of the two-band model. We investigate the effect of the coexistence of a dynamic polaronic lattice distortion with superconductivity on the superconducting transition temperature T_c. In addition we admit for anisotropic pairing and the mixing of d- and s-wave superconducting order parameters. In all our calculations we start from the assumption that the pairing interactions within the two bands considered are too weak to induce superconductivity separately. Thus we are able to investigate the effect of the interband interactions on anisotropic superconductivity and also show how much a polaronic distortion can influence superconductivity.

The two band Hamiltonian we consider, in already condensed form, reads:

$$H = H_0 + H_1 + H_2 + H_{12} \tag{1}$$

$$H_0 = \sum_{k_1\sigma} \xi_{k_1} c^+_{k_1\sigma} c_{k_1\sigma} + \sum_{k_2\sigma} \xi_{k_2} d^+_{k_2\sigma} d_{k_2\sigma} \tag{1a}$$

$$H_1 = -\sum_{k_1 k_1' q} V_1(k_1, k_1') c^+_{k_1+q/2\uparrow}\ c^+_{-k_1+q/2\downarrow}\ c_{-k_1'+q/2\downarrow} \times c_{k_1'+q/2\uparrow} \tag{1b}$$

$$H_2 = -\sum_{k_2 k_2' q} V_2(k_2, k_2') d^+_{k_2+q/2\uparrow}\ d^+_{-k_2+q/2\downarrow}\ d_{-k_2'+q/2\downarrow} \times d_{k_2'+q/2\uparrow} \tag{1c}$$

$$H_{12} = -\sum_{k_1 k_2 q} V_{12}(k_1, k_2) \Big\{ c^+_{k_1+q/2\uparrow}\ c^+_{-k_1+q/2\downarrow}\ d_{-k_2+q/2\downarrow} \times d_{k_2+q/2\uparrow} + \text{h.c.} \Big\}, \tag{1d}$$

where H_0 is the kinetic energy of the bands $i = 1, 2$ with $\xi_{k_i} = \varepsilon_i + \varepsilon_{k_i} - \mu$. Here ε_i denotes the position of the bands, $\varepsilon_{k_1}, \varepsilon_{k_2}$ are the corresponding energies of c and d band with creation and annihilation operators c^+, c, d^+, d, respectively, and μ is the chemical potential. The pairing potentials $V_i(k_i, k_i')$ are assumed to be represented in factorized form as $V_i(k_i, k_i') = V_i \varphi_{k_i} \psi_{k_i'}$ where $\varphi_{k_i}, \psi_{k_i}$ are cubic harmonics for anisotropic pairing which yields for two dimensions and on-site pairing: $\varphi_{k_i} = 1,\ \psi_{k_i} = 1,$

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extended s-wave: $\varphi_{k_i} = \cos k_x a + \cos k_y b = \gamma_{k_i}$ and d-wave: $\varphi_{k_i} = \cos k_x a - \cos k_y b = \eta_{k_i}$, where a, b are the lattice constants along x and y directions. By performing a BCS meanfield analysis of equation (1) those transform to:

$$H_{red} = \sum_{k_1\sigma} \xi_{k_1} c^+_{k_1\sigma} c_{k_1\sigma} + \sum_{k_2\sigma} \xi_{k_2} d^+_{k_2\sigma} d_{k_2\sigma} + \bar{H}_1 + \bar{H}_2 + \bar{H}_{12} \tag{2}$$

$$\bar{H}_i = -\sum_{k'_i} \left[\Delta^*_{k'_i} c^+_{k'_i\uparrow} c^+_{-k'_i\downarrow} + \Delta_{k'_i} c_{-k'_i\downarrow} c_{k'_i\uparrow} \right] + \sum_{k_i,k'_i} V_i(k_i,k'_i) \langle c^+_{k_i\uparrow} c^+_{-k_i\downarrow} \rangle \langle c_{-k'_i\downarrow} c_{k'_i\uparrow} \rangle \ , \ i = 1,2 \tag{2a}$$

and for $i = 2$ c is replaced by d.

$$\begin{aligned} \bar{H}_{12} = -\sum_{k_1,k_2} \Big[& V_{12}(k_1,k_2) \langle c^+_{k_1\uparrow} c^+_{-k_1\downarrow} \rangle d_{-k_2\downarrow} d_{k_2\uparrow} \\ & + V_{12}(k_1,k_2) \langle d_{-k_2\downarrow} d_{k_2\uparrow} \rangle c^+_{k_1\uparrow} c^+_{-k_1\downarrow} \\ & + V^*_{12}(k_1,k_2) d^+_{k_2\uparrow} d^+_{-k_2\downarrow} \langle c_{-k_1\downarrow} c_{k_1\uparrow} \rangle \\ & + V^*_{12}(k_1,k_2) c_{-k_1\downarrow} c_{k_1\uparrow} \langle d^+_{k_2\uparrow} d^+_{-k_2\downarrow} \rangle \\ & - V_{12}(k_1,k_2) \langle c^+_{k_1\uparrow} c^+_{-k_1\downarrow} \rangle \langle d_{-k_2\downarrow} d_{k_2\uparrow} \rangle \\ & - V^*_{12}(k_1,k_2) \langle c_{-k_1\downarrow} c_{k_1\uparrow} \rangle \langle d^+_{k_2\uparrow} d^+_{-k_2\downarrow} \rangle \Big]. \end{aligned} \tag{2b}$$

Here we assume that $\langle c^+_{k_1+q/2\uparrow} c^+_{-k_1+q/2\downarrow} \rangle = \langle c^+_{k_1\uparrow} c^+_{-k_1\downarrow} \rangle \delta_{q,0}$ and equivalently for the d operators. In addition the following definitions are introduced: $\Delta_{k'_i} = \sum_{k_i} V_i(k_i,k'_i) \langle c^+_{k_i\uparrow} c^+_{-k_i\downarrow} \rangle$ together with:

$$A_{k_1} = \sum_{k_2} V_{12}(k_1,k_2) \langle d^+_{k_2\uparrow} d^+_{-k_2\downarrow} \rangle,$$
$$B_{k_1} = \sum_{k_2} V_{12}(k_1,k_2) \langle c^+_{k_2\uparrow} c^+_{-k_2\downarrow} \rangle$$

and $V*_{12} = V_{12}$.

Applying the standard technique we obtain:

$$\langle c^+_{k_1\uparrow} c^+_{-k_1\downarrow} \rangle = \frac{\bar{\Delta}_{k_1}}{2E_{k_1}} \tanh \left[\frac{\beta E_{k_1}}{2} \right] = \bar{\Delta}_{k_1} \Phi_{k_1} \tag{3a}$$

$$\langle d^+_{k_2\uparrow} d^+_{-k_2\downarrow} \rangle = \frac{\bar{\Delta}_{k_2}}{2E_{k_2}} \tanh \left[\frac{\beta E_{k_2}}{2} \right] = \bar{\Delta}_{k_2} \Phi_{k_2} \tag{3b}$$

with $E^2_{k_1} = \xi^2_{k_1} + |\bar{\Delta}_{k_1}|^2$, $\bar{\Delta}_{k_1} = \Delta_{k_1} + A_{k_1}$ and $E^2_{k_2} = \xi^2_{k_2} + |\bar{\Delta}_{k_2}|^2$, $\bar{\Delta}_{k_2} = \Delta_{k_2} + B_{k_2}$. From this we obtain the selfconsistent set of equations:

$$\bar{\Delta}_{k_1} = \sum_{k'_1} V_1(k_1,k'_1) \bar{\Delta}_{k'_1} \Phi_{k'_1} + \sum_{k_2} V_{1,2}(k_1,k_2) \bar{\Delta}_{k_2} \Phi_{k_2} \tag{4a}$$

$$\bar{\Delta}_{k_2} = \sum_{k'_2} V_2(k_2,k'_2) \bar{\Delta}_{k'_2} \Phi_{k'_2} + \sum_{k_1} V_{1,2}(k_1,k_2) \bar{\Delta}_{k_1} \Phi_{k_1} \tag{4b}$$

from which the temperature dependences of the gaps and the superconducting transition temperature have to be determined. If the interactions V are constants, the resulting gaps are momentum independent. A more interesting case is obtained by assuming the following general momentum dependence of the intraband interactions: $V_i = g^{(i)}_0 + g^{(i)}_\gamma \gamma_k \gamma_{k'} + g^{(i)}_\eta \eta_k \eta_{k'}$ where the first term yields onsite pairing, the second extended s-wave pairing, and the last term d-wave pairing. In our calculation we assume that V_1 is proportional to g_0 while V_2 is either determined by g_0 or by g_η. In addition the two bands considered are 1-dimensional in the case of the c bands while the d-related band is 2-dimensional with the following dispersion: $\varepsilon_{k_2} = -2t(\cos k_x a + \cos k_y b)$. The choice of these two bands, which are already p-d hybridised, is dictated from band structure calculations for cuprates [16] where mostly a second nearest neighbour hopping term is included for the in-plane band whereas the out-of-plane band has only minor hybridisations with the in-plane band which arises from plane buckling [16]. This term is neglected here, but becomes effective with finite interband interactions. The plane related Fermi surface is thus a square which becomes rounded off by including the second nearest neighbour hopping term. We have checked the importance of this hopping term to our analysis given below and found that it has nearly no effect on the results. In order to apply the model also to MgB_2 the in-plane hopping has to be modified to account for the hexagonal layer structure whereas the band perpendicular to it is three-dimensional [17]. Here extensions of the above approach are required in order to compare the results in quantitative way also with MgB_2.

As already outlined earlier, throughout this paper we choose our values for the intraband interactions such that both bands separately do not exhibit superconductivity. Specifically, $V_1 = V_2 = 0.01$, where $V_1 = \tilde{V}_1 N_s$, $V_2 = \tilde{V}_2 N_d$. Within this scenario the selfconsistent set of equations is solved numerically as a function of $V_{12} = \tilde{V}_{12}\sqrt{N_s N_d}$, where N_s, N_d are the density-of-states of bands 1, 2, respectively. The results are shown in Figure 1 where both cases $V_2 \sim g_0$ and $V_2 \sim g_\eta$ are considered. In both cases small values of V_{12} are sufficient to induce superconductivity. With increasing V_{12} dramatic enhancements of T_c are obtained which easily exceed 100 K. Interestingly the d-wave component in the two component systems has an additional T_c-increasing factor which increases with increasing interband coupling strength.

This finding demonstrates that a mixed order parameter symmetry favours superconductivity, as opposed to two onsite pairing interactions. It has to be mentioned here, that a mixed order parameter symmetry is not possible on a cubic lattice, but that an orthorhombic distortion has to be considered. By choosing a 10% orthorhombicity an additional small enhancement of T_c as compared to cubic symmetry is obtained, but the general results are overall not affected.

The related superconducting energy gaps are shown in Figure 2 with $V_{12} = 0.5$. Here again the effect of onsite couplings only depresses the gaps as compared to s/d-wave

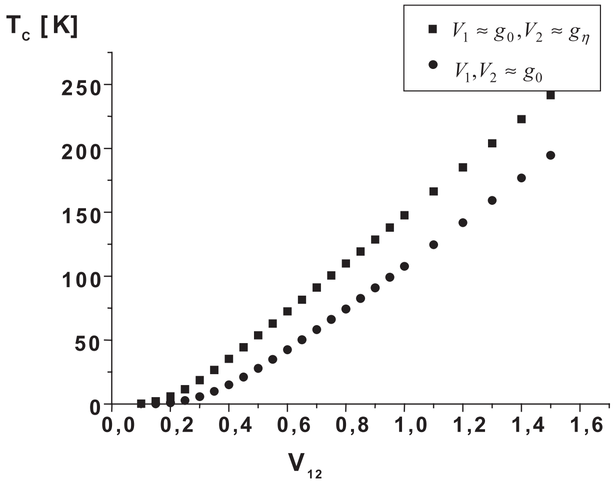

Fig. 1. The dependence of the superconducting transition temperature on the interband coupling V_{12} for the case of both, V_1 and $V_2 \sim g_0$ (circles) and the case where $V_1 \sim g_0$, $V_2 \sim g_\eta$ (squares).

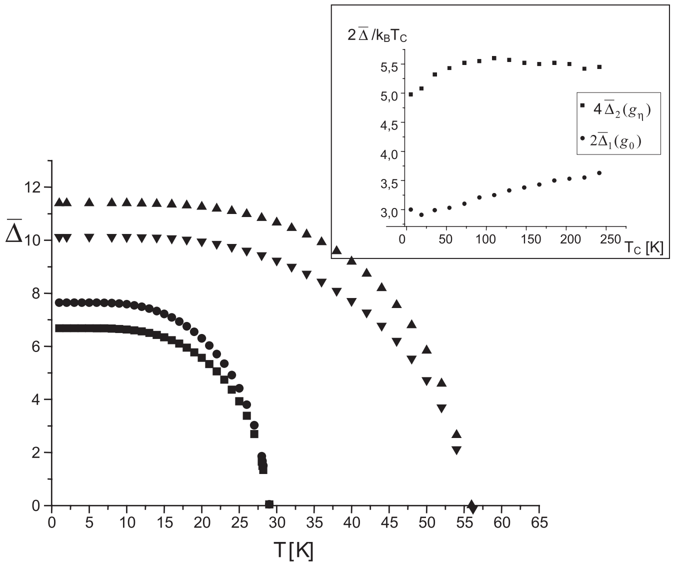

Fig. 2. Temperature dependences of the superconducting gaps in meV. Squares and circles refer to $\bar{\Delta}_1(g_0)$, $\bar{\Delta}_2(g_0)$, while down and up triangles are derived for $\bar{\Delta}_2(g_\eta)$, $\bar{\Delta}_1(g_0)$. The insert shows for the latter case the ratios of the maximal gaps to T_c versus T_c which is equivalent to varying V_{12}. The parameters used throughout the paper are given in [19].

coupled gaps, and in addition a strong anisotropy of the two gaps is observed within the mixed order parameter system. In the insert the ratio of the gaps with respect to T_c is shown as a function of T_c for the mixed order parameter case only. Interestingly the s-wave gap ratio is close to the BCS ratio, slightly increasing with increasing T_c. The corresponding ratio of the d-wave gap is enhanced, as compared to a one band approach, and remains nearly constant as a function of T_c with a slight decrease at small T_c's. The gap versus temperature behaviour is

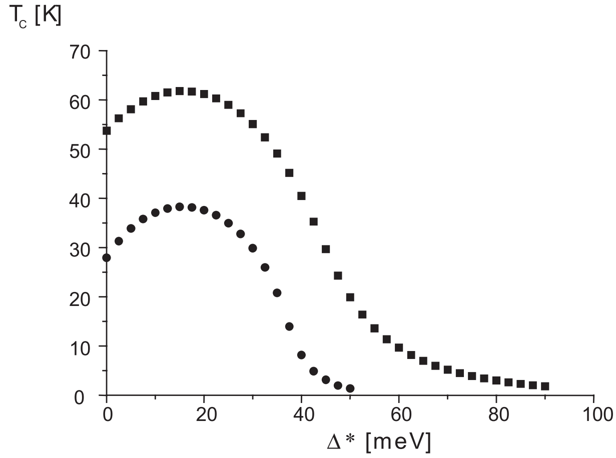

Fig. 3. The dependence of T_c on the polaronic shift Δ^*. The squares refer to s-d coupled order parameters, while the circles correspond to the s-s coupled case.

comparable to the conventional two-band model and follows a BCS type temperature dependence.

Finally we have investigated the question of how the coexistence of dynamic polaronic lattice distortion with superconductivity influences T_c. We start with the assumption that for temperatures $T \gg T_c$ a strong coupling of the one-dimensional electronic band to phonons with momentum q-dependent energy $\hbar\omega$ takes place. This corresponds to modifying the first part of equation (1a) as:

$$\bar{H}_0 = \sum_{k_1\sigma} \xi_{k_1} c^+_{k_1\sigma} c_{k_1\sigma} + \sum_q \hbar\omega_q b^+_q b_q + \frac{1}{\sqrt{2N}} \sum_{q,\sigma,k_1} g(q) c^+_{k_1+q\sigma} c_{k_1\sigma} (b_q + b^+_{-q}). \quad (5)$$

Here b^+, b are phonon creation and annihilation operators and $g(q)$ is the electron-phonon coupling. Following the procedure of reference [18] the k_1-related electronic energies are renormalized by the electron phonon coupling as: $\tilde{H}_0 = \sum_{k_1\sigma} (\xi_{k_1} - \Delta^*) c^+_{k_1\sigma} c_{k_1\sigma}$ with $\Delta^* = \frac{1}{2N} \sum_q (\hbar\omega_q)^{-1} |g(q)|^2$. The transformation to small polarons yields an additional exponential reduction in the hopping integrals which is not relevant for the one dimensional band considered here, but has to be included if similar effects were discussed for the two dimensional band. The polaronic induced density-density attraction has been absorbed in the coupling constant V_1. The q-dependence of the electron-phonon coupling together with that of the level shift have been treated here as integrated averaged quantities but they are explicitly taken into account in reference [20]. Including these modifications of the one dimensional electronic band in the calculation of T_c, and considering again the above two cases, the results shown in Figure 3 are obtained. The polaronic band shift Δ^* first increases T_c enormously but then depresses its value to zero with increasing band shift Δ^*. Since the magnitude of Δ^* depends on the electron-phonon coupling our results show that small and intermediate coupling polaronic distortions lead to a pronounced increase in T_c but reduce T_c in the strong coupling limit. Physically this situation corresponds to an interplay between the interband coupling favouring superconductivity and the lattice distortion which promotes localization. Again a strong enhancement of T_c is observed for the case of two different order parameters as compared to the two s-wave order parameter case.

In conclusion, we have investigated new aspects of the two-band model for superconductivity by considering the influence of different order parameter symmetries on T_c and by studying the effect of a polaronic distortion on it. Combining s and d-wave order parameters always enhances T_c substantially as compared to two isotropic order parameters, since here low energy scales appear from the d-wave channel. The interband coupling also enhances T_c substantially and even at moderate coupling T_c values >100 K are obtained. A polaronic distortion favours superconductivity as long as the corresponding electron-phonon interaction is not too large. For intermediate to large values of the coupling, superconductivity is rapidly depressed. The interesting case of the coexistence of superconductivity with a charge density wave instability within the above discussed scenario will be presented elsewhere together with the discussion of the effect of band narrowing on T_c. Our model with the above given choice of bands is thought to be applicable to cuprates but has to be modified when modelling MgB_2 since here a more complex band structure scheme applies. However, the results indicate clearly that the coupling of two isotropic order parameters, which is realized in MgB_2 limits T_c in agreement with experimental observations.

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