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

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The two-band model as introduced by Suhl, Matthias and Walker [Suhl *et al.*: Physical Review Letters **3**, 551 (1959)] accounts for multiple energy bands in the vicinity of the Fermi energy which could contribute to electron pairing in superconducting systems. 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. Here the effect of the coexistence of a dynamic polaronic lattice distortion with superconductivity on the superconducting transition temperature T_c is investigated. In addition anisotropic pairing and the mixing of *d*- and *s*-wave superconducting order parameters is admitted. In all calculations it is assumed that the pairing interactions within the two bands considered are too weak to induce superconductivity. Thus it is possible to investigate the effect of the interband interactions on anisotropic superconductivity and also to show in how much a polaronic distortion can influence superconductivity. The two band Hamiltonian considered here, in already condensed form, reads:

$$
\begin{aligned}
H &= H_0 + H_1 + H_2 + H_{12} \qquad (1)\\
H_0 &= \sum_{k_1\sigma} \xi_{k_1} c^+_{k_1\sigma} c_{k_1\sigma} + \sum_{k_2\sigma} \xi_{k_2} d^+_{k_2\sigma} d_{k_2\sigma}\\
H_1 &= \sum_{k_1 k_1' q} V_1(k_1, k_1') c^+_{k_1+\frac{q}{2}\uparrow} c^+_{-k_1+\frac{q}{2}\downarrow} c_{-k_1'+\frac{q}{2}\downarrow} c_{k_1'+\frac{q}{2}\uparrow}\\
H_2 &= \sum_{k_2 k_2' q} V_2(k_2, k_2') d^+_{k_2+\frac{q}{2}\uparrow} d^+_{-k_2+\frac{q}{2}\downarrow} d_{-k_2'+\frac{q}{2}\downarrow} d_{k_2'+\frac{q}{2}\uparrow}\\
H_{12} &= \sum_{k_1 k_2 q} V_{12}(k_1, k_2) \{ c^+_{k_1+\frac{q}{2}\uparrow} c^+_{-k_1+\frac{q}{2}\downarrow} d_{-k_2+\frac{q}{2}\downarrow} d_{k_2+\frac{q}{2}\uparrow}\\
&\qquad + h.c. \} \; ,
\end{aligned}
$$

where H_0 is the kinetic energy of the bands $\mathrm{i} = 1, 2$ with $\xi_{k_i} = \varepsilon_i + \varepsilon_{k_i} - \mu$. Here ε_i denotes the position of the 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 like $V_i(k_i, k_i') = V_i \varphi_{k_i} \psi_{k_i}$ where $\varphi_{k_i}, \psi_{k_i}$ are cubic harmonics for anisotropic pairing which yields for dimension $\mathrm{d} = 2$ and on-site pairing: $\varphi_{k_i} = 1$, $\psi_{k_i} = 1$, 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; throughout this paper $a = b$. By performing a BCS meanfield analysis of Eqs.(1) a self-consistent set of coupled gap equations is obtained which has to be solved simultaneously to determine T_c and the temperature dependencies of the gaps. 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: $V_i = g_0^{(i)} + g_\gamma^{(i)} \gamma_k \gamma_{k'} + g_\eta^{(i)} \eta_k \eta_{k'}$ where the first term yields onsite pairing, the second extended *s*-wave pairing and the last term *d*-wave pairing. Here it is assumed 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 one-dimensional in the case of the *c*-bands while the *d*-related band is two-dimensional with the following dispersion:

$$\varepsilon_{k_2} = -2t[\cos(k_x a) + \cos(k_y b)].$$

Throughout the following the values for the intraband interactions are $V_1 = V_2 = 0.01$, where $V_1 = \widetilde{V}_1 N_s$, $V_2 = \widetilde{V}_2 N_d$. Within this scenario the selfconsistent set of equations is solved numerically as function of $V_{12} = \widetilde{V}_{12}\sqrt{N_s N_d}$ where N_s, N_d are the density of states of band 1, 2, respectively. The results are shown in Fig. 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.

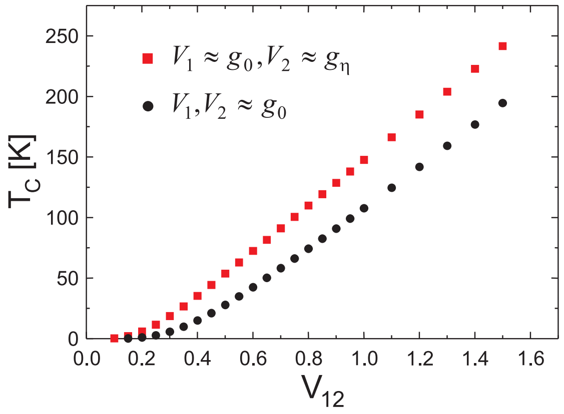

Figure 1: *The dependence of the superconducting transition temperature on the interband coupling V_{12} for the case of both, V_1 and $V_2 \sim g_0$ (circles) and the case where $V_1 \sim g_0$, $V_2 \sim g_\eta$ (squares).*

This finding clearly shows that a mixed order parameter symmetry favors superconductivity, as opposed to two onsite pairing interactions.
In order to determine the possible coexistence of dynamic polaronic lattice distortion with superconductivity it is assumed 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 Eq.(1) as:

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

Here b^+, b are phonon creation and annihilation operators and $g(q)$ is the electron-phonon coupling. Following previous work the k_1 related electronic energies are renormalized by the electron phonon coupling as:

$$\widetilde{H}_0 = \sum_{k_1\sigma} (\xi_{k_1} - \Delta^\star) c_{k_1\sigma^+} c_{k_1\sigma} ,$$

with $\Delta^\star = g(q_0) \frac{2}{\sqrt{N}} \langle b^+_q \rangle \delta_{q,q_0}$, where q_0 is the wave vector which characterizes the width of the polaron induced distortion. 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 Fig. 2 are obtained. The polaronic band shift $\Delta^\star$ first increases T_c enormously but then depresses its value to zero with increasing band shift $\Delta^\star$. Since the magnitude of $\Delta^\star$ depends on the electron-phonon coupling the 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 favoring superconductivity and the lattice distortion which causes 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.

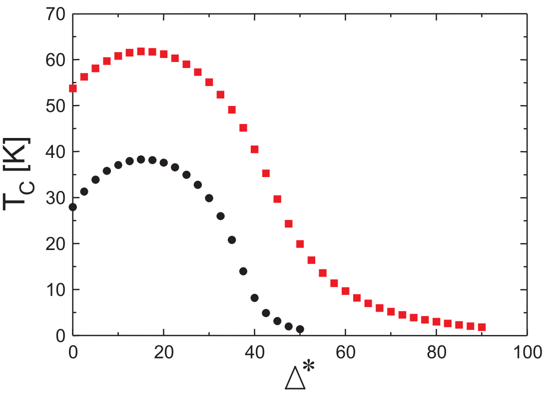

Figure 2: *The dependence of T_c on the polaronic shift $\Delta^\star$. The squares refer to s-d coupled order parameters, while the circles correspond to the s–s coupled case.*

In conclusion, new aspects of the two-band model for superconductivity have been investigated 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 favors 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 and even vanishes for too strong couplings.