T_c enhancement in superconductor and spin-density-wave coexistence

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The interplay of superconductivity and spin-density waves in a two-band system with imperfect nesting and interband coupling is analyzed. Within this model, enhancement of the superconducting critical transition temperature is found. The influence of the interband coupling on this enhancement is presented in detail. The possible connections with the high-T_c oxidic systems are also discussed. The obtained curves of T_c versus the excess carrier concentration fit well with both La-Ba-Cu-O and Y-Ba-Cu-O cases.

Recently, because of the high-T_c oxidic systems, the old[1] problem of the interplay between superconductivity and Fermi surface (FS) driven instabilities, such as spin-density waves (SDW) or (due to the metal-insulator transition[2]), charge-density waves (CDW),[3,4] became of great interest.

Regarding the SDW phase, the exciting new results concern the heavy-fermion,[5] organic,[6] Cr-based,[7] and oxidic[8] superconductors. Related theories take into account instabilities of the normal molecular-orbital states for organic superconductors,[9] antiferromagnetic spin fluctuation and anisotropic order parameters for the heavy-fermion compounds,[10,11] two-band systems for the Cr alloys,[12] and density-of-state (DOS) enhancement for the oxidic superconductors.[13,14] Here we mention the papers of Maki and co-workers,[15] where a detailed analysis of SDW in Bechgaard sales is given.

The general belief concerning the FS driven instabilities supports the idea that they change the electronic spectrum, reducing the critical temperature of the superconducting phase. In contrast to this, the newly obtained results suggest a T_c enhancement due to the coexistence of such instabilities with the superconducting phase. If the nesting condition is accomplished, such a mechanism[4,11,13] does not depend on dimensionality or other detail of the band structure. In fact it is connected to the gap-edge singularities (diverging density of states near the boundary between the CDW or SDW gapped and ungapped region of the FS). A nonsuperconducting gap will cause an effective increase of DOS in the region of the gap edge within the cutoff energy shell around the Fermi energy. This will lead to a T_c enhancement, but only in the case of imperfect nesting.[4,11,13]

In this paper we show that for a multiband system with imperfect nesting, a further T_c enhancement mechanism appears which is strongly related to interband coupling. The possibility of raising T_c by interband scattering was established in the early sixties[16] and it was brought up to date in some aspects in Ref. 17. For these systems it is important to understand that the gained enhancement is due to the fact that in some circumstances the superconducting system can take advantage of a new degree of freedom (like supplementary band or layer indices). This situation occurs in organic superconductors,[18] in layered[19] or $A15$ compounds.[20] In this context, the interband and the interlayer couplings have many similarities.[21] Taking advantage of this fact, a possible T_c enhancement mechanism was suggested in a recent paper.[22] In our case, the effect of the interband scattering on T_c will be much greater, because this scattering will concern those carriers which are closely situated to that region of the FS, where the DOS is increased due to the nonsuperconducting gap edge. So the SDW must be already formed at the Néel temperature $T_N > T_c$.

In order to see this effect, we use a simple 3D model in which two bands are operative at the Fermi level (the extension to multiband case is trivial[16]). The bands are denoted by a and b, and a parameter $\delta\mu$ is used to describe the deviation from the perfect nesting situation. The kinetic energy Hamiltonian in these circumstances will be

$$H_1=\sum_{i,k,\alpha}\xi_i c^{\dagger}_{i,k,\alpha}c_{i,k,\alpha}\,, \tag{1}$$

where i labels the band ($i=a,b$), and $\xi_a=\varepsilon+\delta\mu$, $\xi_b=-\varepsilon+\delta\mu$ with $\varepsilon=k^2/2m$. In fact, $\delta\mu$ is connected to the concentration of the carriers within the system and is related to the deviation of the carrier concentration (δN) from the concentration value (N_0) describing the half-filled band case ($\mu=0$), i.e., $\delta N=N-N_0$. The second Hamiltonian term is a generalized form of the BCS one, so it can be described by the interband and intraband BCS coupling, with different coupling constants λ_{ij},

$$H_2=\tfrac{1}{2}\sum_{i,j,k}\sum_{\alpha,\beta}\lambda_{ij}c^{\dagger}_{i,k,\alpha}c^{\dagger}_{j,-k,\beta}c_{j,-k,\beta}c_{i,k,\alpha}\,, \tag{2}$$

where i,j are the band indices. We used for the superconducting order parameter the Δ_{ij} notation, with $i=j$ for intraband-singlet (λ_{aa} and λ_{bb} are assumed to be equal) and $i\neq j$ for the interband-singlet pairing. The interaction λ_{ij} in our model may correspond either to the phonon or to the nonphonon pairing mechanism. Third, we take into account that due to a magnetic interaction g (see Ref. 23), a SDW pairing can appear within the system[24]

$$H_3=\sum_{\substack{i,j\\(i\neq j)}}\sum_{k,k'}\sum_{\alpha,\beta,\gamma,\delta}g\sigma_{\alpha,\beta}\sigma_{\gamma,\delta}(c^{\dagger}_{i,k,\alpha}c_{j,k,\beta}c^{\dagger}_{j,k',\gamma}c_{i,k',\delta}+\text{H.c.})\,, \tag{3}$$

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which is characterized by the $\Delta_{\mathrm{SDW}} = \Delta_S$ order parameter. $\sigma_{\alpha,\beta}$ denotes the Pauli matrices. (We do not take into account anisotropic SDW order parameters[25] during this analysis.)

In our previous paper,[12] we demonstrated that under these circumstances and considering $\Delta_{ij}^{\alpha,\beta} = \Delta_{ji}^{\alpha,\beta}$, the Gor-kov equations of motion allow two energetically stable coexistence phases. The general characteristics of the coexistence at $T=0$ and a comprehensive analysis of the first ($\Delta = \Delta_{aa} = -\Delta_{bb} \neq 0$, $\Delta_{ab}=0$, $\Delta_S \neq 0$) coexistence phase at $T \neq 0$ was presented.[12] It was found that this phase with vanishing interband order parameter is appropriate for the Cr-Re and Cr-Ru alloys. The predicted T_c square dependence on the Re or Ru concentration was experimentally demonstrated.[26] Hereafter, we take into account the interband scattering, and make a brief analysis of the second coexistence phase, where $\Delta = \Delta_{aa} = \Delta_{bb} \neq 0$, $\Delta_{ab} \neq 0$, $\Delta_S \neq 0$. This analysis, in view of the T_c enhancement possibilities, becomes timely.[27]

The characteristic coupled order-parameter equations, which will be analyzed, are the following:

$$1 = \lambda \sum_{\sigma=\pm} [I_1^\sigma + \delta\mu\,\tilde{\Delta}(\sigma) I_2^\sigma] , \tag{4}$$

$$\Delta_S = g \sum_{\sigma=\pm} \sigma[\Delta_\sigma I_1^\sigma - \Delta_{ab}\tilde{\Delta}(\sigma) I_2^\sigma] , \tag{5}$$

$$\Delta_{ab} = |\lambda_{ab}| \sum_{\sigma=\pm} \left[\frac{\delta\mu}{\delta\tilde{\mu}} \tilde{\Delta}(\sigma)\tilde{\Delta}_\sigma I_2^\sigma - \frac{\Delta_{ab}}{\delta\tilde{\mu}} I_3^\sigma \right] , \tag{6}$$

$$n = \sum_{\sigma=\pm} \{ I_3^\sigma - [\tilde{\Delta}^2(\sigma) - \Delta^2] I_3^\sigma \} . \tag{7}$$

In Eq. (7), $n = \delta N / 4N(0)$. In fact, the presence of n is due to $\delta\mu$; $\delta\mu = 0$ implies $n=0$. Concerning the high-T_c superconductors, both La_2CuO_4 and $YBa_2Cu_3O_{6.5}$ contain only divalent copper. Superconductivity will emerge only if the copper is oxidized higher than the divalent state. This is accomplished by a carrier-concentration modification in the Cu—O antibonding band,[28] i.e., a contribution in n. In $La_{2-x}(Sr,Ba)_xCuO_{4-y}$ this is realized by doping with divalent Sr or Ba, while the same effect is obtained by increasing the oxygen content y, in $YBa_2Cu_3O_{6.5+y}$. In the first case, n is related to (a monotonic function of) $1 - N_e/N_s = x - 2y$ (Ref. 29) (where the e and s subscript refer to electron and site, respectively) and for the second case to y [similarly for the Bi-based 2:2:1:2 (Ref. 30) and Tl-based 2:1:2:2 (Ref. 31) compounds]. The notations used in Eqs. (4)–(7) are

$$I_1^\sigma = \frac{1}{2} \sum_k \sum_{\nu=\pm} \frac{E_\sigma + \nu\,\delta\mu}{\omega_\nu(\sigma) E_\sigma} \tanh\left[\frac{\beta}{2} \omega_\nu(\sigma) \right] , \tag{8}$$

$$I_2^\sigma = \frac{1}{2} \sum_k \sum_{\nu=\pm} \frac{\nu}{\omega_{-\nu}(\sigma) E_\sigma} \tanh\left[\frac{\beta}{2} \omega_{-\nu}(\sigma) \right] , \tag{9}$$

$$I_3^\sigma = \frac{1}{2} \sum_k \sum_{\nu=\pm} \frac{E_\sigma + \nu\,\delta\mu}{\omega_\nu(\sigma)} \tanh\left[\frac{\beta}{2} \omega_\nu(\sigma) \right] , \tag{10}$$

where $\beta = 1/k_B T$, $E_\sigma^2 = \varepsilon^2 + \Delta_{ab}^2$, $\omega_\pm^2(\sigma) = (E_\sigma \pm \delta\tilde{\mu})^2 + \tilde{\Delta}^2(\sigma)$, and $(\delta\tilde{\mu})^2 = (\delta\mu)^2 + \Delta_{ab}^2$. The renormalized gaps are defined as $\tilde{\Delta}(\sigma) = (\delta\mu\,\Delta - \Delta_{ab}\Delta_\sigma)/\delta\tilde{\mu}$ and $\tilde{\Delta}_\sigma = (\delta\mu\,\Delta_\sigma + \Delta_{ab}\Delta)/\delta\tilde{\mu}$, with $\Delta_\sigma = \sigma\Delta_S$. The order parameters for the pure phases are $\Delta_0 = 2\Omega \exp[-1/\lambda N(0)]$, and $\Delta_{S0} = 2\Omega \exp[-1/gN(0)]$. Where Ω is the cutoff energy and $N(0)$ is the unperturbed density of states at the Fermi level. The corresponding critical transition temperatures are $T_{c0} = \gamma\Delta_0/\pi k_B$ and $T_{N0} = \gamma\Delta_{S0}/\pi k_B$, with $\gamma = 1.781$.

At $T=0$, by crossing the phase separation line [the phase diagram was constructed in the ($y = \Delta_{S0}/2n$, $x = \Delta_0/2n$) plane] between the BCS and the analyzed coexistence phase, the superconducting gap $\Delta(T=0)$ will increase as compared to Δ_0.[32]

At $T \neq 0$, in the high-temperature region, where only the SDW exists, the results were already presented.[12] At low temperatures, in the coexistence domain, all the gap equations must be simultaneously treated. Just below T_c the $\Delta_S(T)$ expression becomes

$$\Delta_S(T) = \tilde{\Delta}_{S0} - (2\pi\tilde{\Delta}_{S0} k_B T)^{1/2} \exp\left[-\frac{\Delta_{S0}}{k_B T} \left[1 + \frac{\Delta^2}{(\delta\mu)^2 - \Delta_{S0}^2} + \frac{\Delta_{S0}^2 \Delta_{ab}^2}{(\delta\mu)^2[(\delta\mu)^2 - \Delta_{S0}^2]} \right] \right] \cosh\left[\frac{\delta\mu}{k_B T} \right] , \tag{11}$$

where $\tilde{\Delta}_{S0} = [\Delta_{S0}(\Delta_{S0} - 2n)]^{1/2}$ and the superconducting gaps Δ and Δ_{ab}, in the same temperature region (and being $\Delta_S \ll [(\delta\mu)^2 - \Delta_S^2]^{1/2}$, are

$$\Delta(T) = k_B T_c \frac{2\sqrt{2}\pi}{\sqrt{3}} \frac{\delta\mu}{[(\delta\mu)^2 - \Delta_S^2]^{1/2}} \left[1 - \frac{T}{T_c} \right]^{1/2} , \tag{12}$$

$$\Delta_{ab}(T) = k_B T_c \frac{2\pi}{\sqrt{3}} \frac{\Delta_S}{[(\delta\mu)^2 - \Delta_S^2]^{1/2}} \left[1 - \frac{T}{T_c} \right]^{1/2} . \tag{13}$$

In order to given an analytical expression for T_c, we consider $|\lambda_{ab}| N(0) \ll 1$, and two limiting cases, namely, for $\Delta_S \ll \Omega \ll (\delta\mu^2 - \Delta_S^2)^{1/2}$, we have

$$T_c = T_{c0} \exp\left[-\frac{|\lambda_{ab}|}{\lambda} \frac{\tilde{\Delta}_{S0}^2}{(\Delta_{S0} - n)^2} \ln\left[\frac{\Delta_{S0}}{\Delta_0} \right] \right] , \tag{14}$$

and for $\Delta_S \ll (\delta\mu^2 - \Delta_S^2)^{1/2} \ll \Omega$, it is obtained

$$T_c = T_{c0} \frac{\delta\mu + \Delta_S}{\Delta_S} \exp\left[\frac{\delta\mu^2}{\Delta_S^2} \frac{1}{|\lambda_{ab}| N(0)} \right] . \tag{15}$$

As it can be seen from Eq. (14), T_c is smaller than T_{c0}. Therefore, in this case interband effect is not so important, from the point of view of the T_c enhancement possibilities. Though, in the second case of large cutoff energy, T_c is much greater than T_{c0}, and the critical transition temperature is strongly influenced by $\delta\mu$. This fact suggests that an extended analysis of the T_c values must be done in this situation. For this we wrote, in a form suitable for numerical computation, the exact equation of T_c, which can be obtained, after some algebra, from Eqs. (4)–(7):

$$\Lambda = \frac{\Delta_S^2(T_c)}{[\delta\mu(T_c)]^2} l - \frac{n}{\delta\mu(T_c)} . \tag{16}$$

Computing $\Delta_S(T)$ and $\delta\mu(T)$ functions from Eqs. (5) and

(7) at a fixed n (being at T_c we put $\Delta=\Delta_{ab}=0$), T_c can be obtained from Eq. (16) for a given Λ and l value. We used the notation $\Lambda=1/|\lambda_{ab}|N(0)$ and $l=\ln(T_{N0}/T_{c0})$. In Fig. 1, in the domain situated between curve 1 and the $n/\Delta_{S0}=0.56$ straight line for every Λ, n, and (all possible) l values the obtained T_c was always greater than T_{c0}. This holds also for the second domain, which is situated below curve 2, the curve on which the maximum T_c values can be obtained for a given n. Furthermore, we emphasize the following: (i) a reentrant superconducting phase is obtained for $0.50<n/\Delta_{S0}<0.56$ (which cannot be found at $T=0$), (ii) T_c will increase if l (i.e., the strength of the magnetic correlation g) or $|\lambda_{ab}|N(0)$ is rising, (iii) the enhancement of T_c can be *very great*; the coupled gap equations allow a coexistence solution with $T_c \simeq T_{N0}$ (usually $T_{N0}\sim 300$ K), (iv) even relatively small $|\lambda_{ab}|N(0)$ values (~ 0.1) which give relatively high critical temperatures, $T_c \sim 30T_{c0}$ (see Fig. 2).

In terms of concentrations n, the analyzed coexistence phase exists only if n is situated between two critical concentration values, $n_{c1}<n<n_{c2}$. As n increases, T_c reaches its maximum near n_{c2} and drops abruptly. The n_{c1} value can be expressed without any approximation: $n_{c1}=\Delta_{S0}\{[1+4l(1-\Lambda)]^{1/2}+2(\Lambda-l)-1\}/2(\Lambda-l)$ for the $4l(l-\Lambda)+1>0$ case (otherwise $n_{c1}=0$). For $\Lambda=1$ the value of n_{c1} is $\Delta_{S0}[2+l/(l-\Lambda)]^{-1}$. The expression of n_{c2} being more complicated, we just underline its property of being monotonic function (like n_{c1}) of Λ and l. Our T_c vs n curves (see Fig. 2) are similar to what is obtained for the 2:1:4 and 1:2:3 compounds. For La-Ba-Cu-O a straight line is found,[33,34] so T_c is approximately proportional to the number of the excess carriers, i.e., to n. This situation is illustrated by lines 1 and 3 in Fig. 2. On the other hand, in Y-Ba-Cu-O curves exhibiting an inflexion point are measured,[34,35] as in curves 2, 4, and 5 of Fig. 2. The straight line can be obtained from Eq. (16) for small $|\lambda_{ab}|N(0)$ values [the slope of which is proportional to $|\lambda_{ab}|N(0)$]. Increasing the interband coupling, we obtain greater T_c values (as in 1:2:3 compounds) and the curves will change slightly; near n_{c1}, T_c is proportional

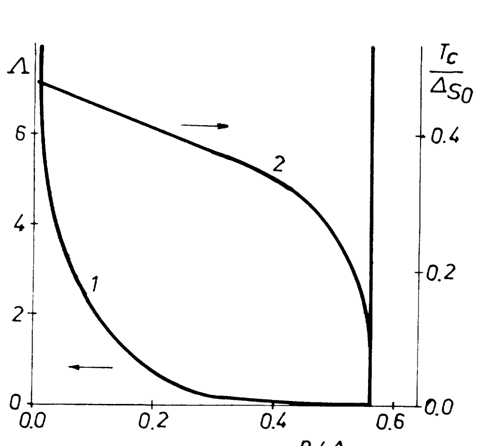

FIG. 1. The region where $T_c > T_{c0}$ is situated between curve 1 and the vertical straight line ($n/\Delta_{S0}=0.56$). The maximum T_c/Δ_{S0} values which can be obtained for a given n/Δ_{S0} are represented with curve 2.

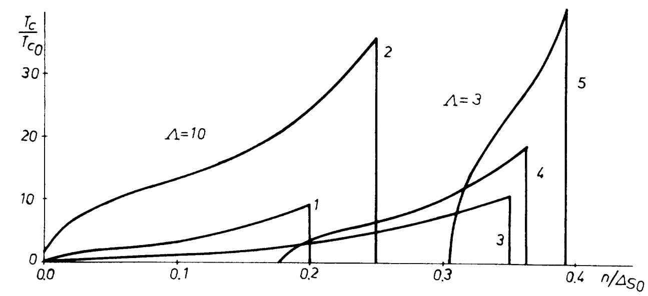

FIG. 2. T_c/T_{c0} ratio vs n/Δ_{S0} for fixed Λ and T_{N0}/T_{c0} values, for curve 1 ($\Lambda=10$ and $T_{N0}/T_{c0}=12$); curve 2 ($\Lambda=10$ and $T_{N0}/T_{c0}=50$); curve 3 ($\Lambda=3$ and $T_{N0}/T_{c0}=18$); curve 4 ($\Lambda=3$ and $T_{N0}/T_{c0}=28$); curve 5 ($\Lambda=3$ and $T_{N0}/T_{c0}=70$).

with $(n-n_{c1})^{1/2}$ and an inflexion point will appear [as it can be checked by performing the second derivative of Eq. (16)] due to the change in slope of the Δ_S vs n curve.

In conclusion, we demonstrated that a T_c enhancement due to an SDW with imperfect nesting in a two-band system (with the possibility of extending to the multiband case) is really possible. The presence of antiferromagnetic correlations in 2:1:4 (Refs. 36 and 37) and 1:2:3 (Refs. 37 and 38) compounds is already established. It is believed that a spin-density wave (whose period is commensurate with that of the lattice[39]) is responsible for the high T_c, as it was found recently,[40] via a linear-muffin-tin-orbital atomic-sphere-approximation (LMTO-ASA) self-consistent spin-polarized calculation in the CuO_2 planes. Even in the newly discovered Bi-based compounds, instabilities (of spin-density-wave type) may be related to the FS.[41] Knowing that the oxidic compounds are multiband systems and that the coexistence phase with antiferromagnetism in these systems will have lower energy than superconductivity alone,[42] our model could have important implications in this field.

Note added. Recent measurements reported by Lee *et al.* [Phys. Rev. B **37**, 2285 (1988)] for $R_1Ba_2Cu_3O_{7-\delta}$ (where R denotes the rare-earth elements Nd, Sm, Eu, Gd, Dy, Ho, Er, Tm, Yb, and Lu) indicates that the thermoelectric power S can have either a positive or negative sign. This confirms the measured positive S of Cava *et al.* [Phys. Rev. Lett. **58**, 1574 (1987)] and Cooper *et al.* [Phys. Rev. B **35**, 8794 (1987)], and the negative S of Khim *et al.* [Phys. Rev. B **36**, 2305 (1987)]. These observations underline the multiband nature of the oxidic superconductors, with partially filled electron and hole bands, and with a slight shift in the Fermi energy due to excessive oxygen deficiency (see Lee *et al.*). Exactly as we modeled the electronic band structure, by considering for the two bands $\xi_a=\varepsilon+\delta\mu$ and $\xi_b=-\varepsilon+\delta\mu$. The thermoelectric power will change due to the change in occupation of the electron band and hole band.

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[28]For a good review of these problems, see *Proceedings of the Adriatico Research Conference on High-Temperature Superconductivity, Trieste, 1987,* edited by S. Lundqvist, E. Tosatti, M. P. Tosi, and Yu Lu (World Scientific, Singapore, 1987).

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$$\ln(\Delta_0/\Delta)=\Delta_S[2n(1-4x^2)]^{-1}\times\{1-(1+4x^2)^{-1/2}\ln[(1+\sqrt{1+4x^2})/x]+2|\lambda_{ab}|N(0)\ln^2 x\}$$

changes sign. A similar result was obtained many years ago for the CDW phase: A. I. Rusinov, D. C. Kat, and Yu.V. Kopaev, Zh. Eksp. Teor. Fiz. **65**, 1984 (1973) [Sov. Phys. JETP **38**, 991 (1974)].

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