Enhancement of the superconducting critical temperature in layered compounds

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(Received 27 July 1987)

It is shown that interlayer pairing interaction can enhance the superconducting critical temperature of layered compounds in comparison with the critical temperature of the intralayer processes. Possible implications for high-T_c oxidic superconductors are also discussed.

The study of the superconducting properties of layered structures represents today a classical problem. Its evolution is connected to the hope of finding fluctuation behavior characteristics of a two-dimensional (2D) superconductor,[1] various unusual phenomena for different parameters of the superconducting phase [like the dimensional crossover in the T dependence and the sharp peak in the layer thickness dependence of H_{c2} (Ref. 2)], and remarkable experimental implementations (see, for example, the Nb-based superconducting superlattices[3]). Starting from the papers of Kats[4] and Lawrence and Doniach,[5] most of the theoretical works study the upper critical field,[6] but other characteristics are also analyzed; for example, p-wave superconductivity in layered structures,[7] increase in critical parameters in anisotropic metallic superlattices,[8] thermal conductivity,[9] or exotic mechanisms.[10] The number of studied layered structures increases every year (the last group of substances being the high-T_c oxidic superconductors[11]). The experimental data connected to this field[12] give rise to a very interesting question: Does the critical temperature of layered compounds depend only on intralayer processes, or do other contributions also exist which are connected exclusively to the sandwich characteristics of the studied systems? If the latter type of contributions does exist, then it means that it is possible to modify the critical temperature not only with the intralayer processes but also with the sandwich structure itself. In this paper we try to show that such a "sandwich effect," which enhances T_c, does exist, being closely related to the interlayer coupling (ILC). (The ILC is characteristic of the sandwich, and it does not exist if there is no layered structure.) From the theoretical size, the ILC study is motivated also by the fact that in the strict sense there is no superconducting order in 2D systems.[13]

We will consider on general grounds that a given intralayer mechanism gives rise to a superconducting critical temperature $T_0=\beta_0^{-1}$, and we are interested in finding out to what extent β_0 is modified by ILC. In this paper the microscopic origin of β_0 and ILC is not analyzed in detail;[14] only its presence will be important. We analyze a very simple system consisting of an infinite sandwich formed by identical layers, the nearest neighbors of which are coupled by the same interlayer tunneling (J_{ij}) and biparticular pairing (V_{ij}) interactions.[15] The Hamiltonian we use,

$$H=s\sum_{j,\sigma}\int d^2r\,\psi^\dagger_{j\sigma}(r)\left[-\frac{\nabla^2}{2m}-\mu\right]\psi_{j\sigma}(r)+\frac{s}{2}\int d^2r\sum_{l,j,\sigma}J_{jl}\psi^\dagger_{j\sigma}(r)\psi_{l\sigma}(r)\ ,$$
$$+\frac{s}{2}\sum_{\substack{j,l,\\ \sigma,\sigma'}}\int d^2r\int d^2r'\,\psi^\dagger_{j\sigma}(r)\psi^\dagger_{l\sigma'}(r')V_{jl}(r-r')\psi_{l\sigma'}(r')\psi_{j\sigma}(r)\ , \tag{1}$$

is a classical one,[1,4–9,15] in which the $\psi_{j\sigma}(r)$ field corresponds to a fermion with spin σ in the jth layer, and s is the layer repeat distance. Using Hartree-Fock techniques, we obtain the following Gorkov equations of motion:

$$\begin{aligned}(i\omega_n-\xi_k)G^{\sigma\sigma'}_{jj'}(k)&=\delta_{jj'}\delta_{\sigma\sigma'}+\tfrac{1}{2}\sum_l J_{jl}G^{\sigma\sigma'}_{lj'}(k)+\sum_{l,\alpha}\Delta^{\sigma\alpha}_{jl}(k)F^{+\alpha\sigma'}_{lj'}(k)\ ,\\ (i\omega_n+\xi_k)F^{+\sigma\sigma'}_{jj'}(k)&=-\tfrac{1}{2}\sum_l J_{jl}F^{+\sigma\sigma'}_{lj'}(k)+\sum_{l,\alpha}\Delta^{\sigma\alpha *}_{jl}(k)G^{\alpha\sigma'}_{lj'}(k)\ ,\end{aligned} \tag{2}$$

where k is a two-dimensional quasi-impulse vector, $\xi_k=(k^2/2m)-\mu$, and $G^{\sigma\sigma'}_{jj'}(k)$ and $F^{+\sigma\sigma'}_{jj'}(k)$ are the standard normal and anomalous Green's functions. Taking into account

$$J_{j'j}=J(\delta_{j',j+1}+\delta_{j',j-1})\ ,\qquad V_{j'j}(k)=V_0\delta_{j,j'}+\tfrac{1}{2}V_1(\delta_{j',j+1}+\delta_{j',j-1})\ ,$$

and using a Fourier series transformation with respect to $j-j'$, we obtain the following coupled gap equations (V_0 and

V_1 are considered to be attractive interactions):

$$\Delta_0 = -T\sum_n \int_q V_0 \frac{\Delta(q,q_z)}{(i\omega_n)^2-\varepsilon_q^2-|\Delta(q,q_z)|^2} ,$$

$$\Delta_1 = -T\sum_n \int_q V_1\cos(q_z s) \frac{\Delta(q,q_z)}{(i\omega_n)^2-\varepsilon_q^2-|\Delta(q,q_z)|^2} ,$$

$$\Delta_2 = -T\sum_n \int_q V_1\sin(q_z s) \frac{\Delta(q,q_z)}{(i\omega_n)^2-\varepsilon_q^2-|\Delta(q,q_z)|^2} , \tag{3}$$

where

$$\varepsilon_q = \xi_q + J\cos(q_z s) ,$$

$$\Delta = \Delta_0 + \Delta_1\cos(q_z s) + \Delta_2\sin(q_z s) ,$$

and

$$\int_q = \int \frac{d^2q}{(2\pi)^2}\int_{-\pi/s}^{\pi/s}\frac{dq_z}{2\pi} .$$

It is interesting to mention that becasue of the interlayer coupling V_1, in the gap function there appear q_z-dependent even and odd contributions, where z is the direction perpendicular to the layers. We must mention that Eqs. (3) are perfectly consistent with the gap equations obtained by Klemm and Scharnberg.[7]

First of all we analyze the pure phases (no coexistence). β_0^{-1}, the critical temperature for the $\Delta_0 \neq 0$, $\Delta_1 = \Delta_2 = 0$ phase is given by

$$1 = |V_0| \int_q \frac{1}{2\varepsilon_q}\tanh\left(\frac{\beta_0\varepsilon_q}{2}\right) . \tag{4}$$

The superconducting state caused by interlayer pairing interaction (for example, the singlet type $\Delta_1 \neq 0$, $\Delta_0 = \Delta_2 = 0$) has the critical temperature $\beta_1^{-1} = T_1$, where

$$1 = |V_1| \int_q \frac{\cos^2(q_z s)}{2\varepsilon_q}\tanh\left(\frac{\beta_1\varepsilon_q}{2}\right) . \tag{5}$$

It can be shown that in Eqs. (4) and (5) the critical temperatures are monotonic increasing functions of the coupling constants. Now, if we consider a concrete V_1 value (V_1^0) (in this case β_1 is denoted by β_1^0), so that $V_0 = V_1^0$, from Eqs. (4) and (5) we have

$$\int_q \frac{1}{2\varepsilon_q}\left[\tanh\left(\frac{\beta_0\varepsilon_q}{2}\right) - \cos^2(q_z s)\tanh\left(\frac{\beta_1^0\varepsilon_q}{2}\right)\right] = 0 . \tag{6}$$

To satisfy Eq. (6) we must compensate for the lowering trigonometric function in the second term, and this can be done only by increasing β_1^0 as compared with β_0. Thus $V_0 = V_1^0$ gives $T_1^0 < T_0$, which also means that for $|V_1| \leq |V_0|$ we have $T_1 < T_0$. This means that if the ILC does not exceed V_0, in the case of pure phases, we cannot obtain an enhancement of the system's critical temperature in comparison with T_0. The situation is perfectly similar for the triplet case too, and spectacular effects cannot be obtained even if we take into account intralayer k-dependent biparticular pairing interaction within the system.[7] This is not a promising result in the tentative to obtain high superconducting critical temperature with ILC, because in practice it is hard to obtain practically $|V_1| \gg |V_0|$ (see Refs. 15 and 16).

Besides the pure superconducting phases, Eq. (3) also allows a coexistence solution, $\Delta_0 \neq 0$, $\Delta_1 \neq 0$, $\Delta_2 = 0$. This is connected to the fact that Δ_0 and Δ_1 represent singlet pairing, which gives rise to even k dependence in the gap.[17] The coexistence becomes possible because of the tunneling term $J \neq 0$, which gives

$$I(J,\beta) = \int_q \frac{\cos(q_z s)}{2\varepsilon_q}\tanh\left(\frac{\beta\varepsilon_q}{2}\right) \neq 0 . \tag{7}$$

The critical temperature $T_c = \beta_c^{-1}$ for the coexistence phase is determined by the following equality:

$$\left[1 - |V_0| \int_q \frac{1}{2\varepsilon_q}\tanh\left(\frac{\beta_c\varepsilon_q}{2}\right)\right]\left[1 - |V_1| \int_q \frac{\cos^2(q_z s)}{2\varepsilon_q}\tanh\left(\frac{\beta_c\varepsilon_q}{2}\right)\right] - |V_1|\,|V_0| I^2(J,\beta_c) = 0 . \tag{8}$$

Since $|V_1|\,|V_0| I^2(J,\beta_c) > 0$, to satisfy Eq. (8) we must have a positive value for the product of the first two factors in square brackets in Eq. (8). Supposing that V_1 is a infinitesimally small value, $|V_1| \ll 1$, in order to satisfy Eq. (8), the first square bracket from Eq. (8) must be positive; so

$$1 - |V_0| \int_q \frac{1}{2\varepsilon_q}\tanh\left(\frac{\beta_c\varepsilon_q}{2}\right) > 0 . \tag{9}$$

The comparison between Eqs. (4) and (9) automatically yields $\beta_c < \beta_0$; so

$$T_c > T_0 . \tag{10}$$

In Eq. (10) we obtain a very interesting result which can be summarized in the following terms: An infinitesimally small interlayer coupling can give rise to an even-parity coexistence superconducting phase in layered compounds which has a greater superconducting critical temperature than the superconducting state created by the intralayer mechanisms. This conclusion also stays true for the case in which the intralayer pairing gives rise to a cosine-dependent gap instead of the constant Δ_0.

Equation (10) is written for very small V_1. What happens if V_1 increases, and which is the real size of the T_c enhancement? To answer these questions, we use Eq. (4) in Eq. (8), and explain $1/V_1$ as

$$\frac{1}{-V_1} = \frac{I^2(J,\beta_c)}{\int_q \frac{1}{2\varepsilon_q}[\tanh(\beta_0\varepsilon_q/2) - \tanh(\beta_c\varepsilon_q/2)]} + \int_q \frac{\cos^2(q_z s)}{2\varepsilon_q}\tanh\left(\frac{\beta_c\varepsilon_q}{2}\right) . \tag{11}$$

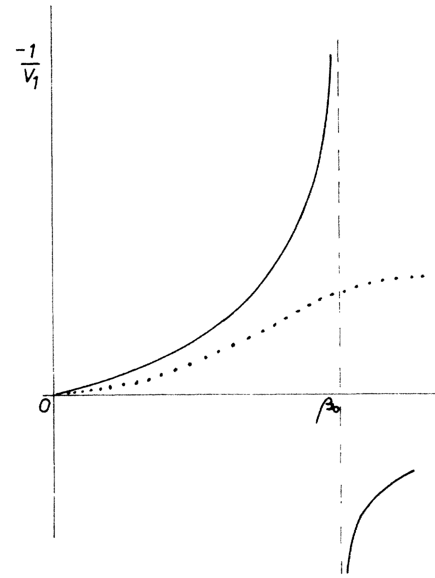

FIG. 1. $1/V_1$ vs $\beta_c = T_c^{-1}$ for the coexistence phase $\Delta_0 \neq 0$, $\Delta_1 \neq 0$, $\Delta_2 = 0$ (continuous line) in arbitrary units. The dotted line represent $1/V_1$ in the case of pure phase $\Delta_1 \neq 0$, $\Delta_0 = 0$, $\Delta_2 = 0$, as deduced from Eq. (5).

The variation of $1/V_1$ vs β_c is plotted in arbitrary units in Fig. 1. [The dotted line represents $1/V_1$ in the pure case; see Eq. (5).] This figure illustrates that T_c is enhanced in comparison with T_0 and T_1 for an arbitrary attractive V_1. The enhancement can be infinitely large, but its actual value depends on the characteristics of the analyzed system. To obtain a concrete image about the possibilities, we make a rough estimation for the $J \ll \mu$ case, and from Eq. (11) we obtain the relation

$$X(T_1)X(T_0) \sim J^2/T_0T_1\,, \tag{12}$$

where $X(T) = (T_c/T)\ln(T_c/T)$ and T_0, T_1 are given in Eqs. (4) and (5). Equation (12) gives, for example, $T_c/T_0 \sim 3$ for $T_0 \sim T_1/10^{-1} \sim 10$ K, $J \sim 10^{-2}$ eV or $T_0 \sim T_1 \sim 10$ K, $J \sim 2\times 10^{-3}$ eV. Even greater values can be obtained (for example, at $T_0 \sim T_1 \sim 10$ K, $J \sim 5\times 10^{-2}$ eV or $T_0 \sim T_1 \sim 30$ K, $J \sim 6\times 10^{-2}$ eV, we have $T_c/T_0 \sim 10$).

In conclusion, we have showed that in a layered structure a critical-temperature enhancement due to interlayer coupling can appear. The condensed phase is of singlet type. One of the possible domains of application of these results could be in the domain of the high-T_c superconducting ceramics, where the importance of the layered structure and of the interlayer coupling has been pointed out recently.[12,18]

Two of the authors (Zs.G. and M.G.) gratefully acknowledge the hospitality of the International Centre of Theoretical Physics, Trieste during the 1987 summer workshop, and of the Central Research Institute of Physics, Budapest during the International Conference on Low-Temperature Physics, November, 1987, where parts of this material were presented and discussed. We also thank Professor A. Glodeanu and Professor P. Fazekas for helpful discussions and comments.

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