PHYSICAL REVIEW B VOLUME 40, NUMBER 1 1 JULY 1989

In-plane impurities in superconducting layered systems

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(Received 24 October 1988)

The influence of the in-layer magnetic and nonmagnetic impurities on the superconducting phases in layered systems is analyzed in detail. It is shown that the critical temperature is strongly depressed by the in-plane nonmagnetic impurities, and this depression can be connected to the presence of the interlayer pairing. The relevance of the deduced results for high-T_c materials is also discussed.

The description of the superconducting properties of layered systems[1] has attracted much attention in the last few years. This is because of their extremely unusual characteristics. For example, superlattices[2] with a sharp peak in the layer-thickness dependence, and a dimensional crossover[3] in the H_{c2} vs T dependence; or the organic superconducting compounds,[4] with bis(ethylenedithio)tetrathiatulvalene donor conducting sheets[5] which exhibit a relatively high critical temperature,[6] or two different superconducting phases.[7] Another unusual property is the Takahashi-Tachiki effect[8] seen in superconducting multilayers.[9] We can add here also the low-T_c materials, such as $Hg_{3-\delta}AsF_6$ (Ref. 10) or $Hg_{3-\delta}SbF_6$,[11] containing planes built up by linear Hg chains, the chains or adjacent planes being perpendicular to each other, with an interesting pressure dependence, which gives[12] three-dimensional (3D) characteristics under pressure annealing. Lastly we mention the high-T_c oxidic materials,[13] with properties which, up to this date, could not be clearly and coherently understood.[14] In order to clarify some aspects of such complex behavior many procedures can be used, one of which is based on chemical substitution and impurity doping.[15–19] The effects obtained, analyzed theoretically, give important information concerning the model and its assumptions:[20] type of pairing,[21] gap symmetry,[22] the influence of the interlayer pairing,[23] the effect of the anisotropic pairing interactions,[24] and also interlayer couplings.[25] Motivated by these considerations, in this paper we will analyze the effects of the in-layer doping in layered superconducting systems (describing here only the even-parity superconducting phase). We will use a standard Abrikosov-Gorkov[26] (AG) mediation procedure over the random in-plane positions of the magnetic and nonmagnetic impurities.

The layered system is considered in the traditional way[1,21,27] by taking into account an infinite sandwich formed from identical layers, the nearest neighbors of which are coupled by interlayer hopping ($J_{i,j}$) and two-particle pairing $[V_{i,j}(r,r'),i\neq j]$ interactions. The individual layers are characterized by the in-layer hopping $[t_i(r,r')]$ and in-layer pairing $[V_{i,j}(r,r'),i=j]$ interactions:

$$H_0=s\sum_{i,\sigma}\int d^2r\int d^2r'\Psi^\dagger_{i,\sigma}(r)[t_i(r,r')-\mu\delta(r-r')]\Psi_{i,\sigma}(r')+\frac{s}{2}\sum_{i,j,\sigma}\int d^2r J_{i,j}\Psi^\dagger_{i,\sigma}(r)\Psi_{j,\sigma}(r)$$
$$+\frac{s}{2}\sum_{i,j,\sigma,\sigma'}\int d^2r\int d^2r'\Psi^\dagger_{i,\sigma}(r)\Psi^\dagger_{j,\sigma'}(r')V_{i,j}(r,r')\Psi_{j,\sigma'}(r')\Psi_{i,\sigma}(r)\,. \quad (1)$$

In Eq. (1) s is the layer repeat distance, r is the two-dimensional position vector, $\Psi^\dagger_{i,\sigma}(r)$ creates a fermion with spin σ at position r in the ith layer, μ is the chemical potential, and

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

In H_0 the intralayer pairing mechanism is described with V_0. We also take into account an interlayer pairing V_1, the importance of which was pointed out for superlattices (especially for light intercalates[21]), organic layered superconductors,[28] and also high-T_c materials.[23,27,29,30] Concerning the interlayer hopping term J, we mention that its destructive effect on the in-plane pairing was recognized fifteen years ago.[31] Furthermore, it becomes clear that J together with the biparticular interlayer interaction V_1 play an essential role in the stabilization of the bulk superconducting phase.[32] The importance of the interlayer hopping was claimed, in fact, many times in different aspects,[33] and recently Griffin,[34] underlining its necessity, showed that the interlayer biparticular (Coulomb-type) interaction is not strong enough to suppress the phase fluctuations sufficiently to stabilize a 2D Bose condensate in each layer.

Besides H_0 we consider the effect of in-layer impurities with a new Hamiltonian term

$$H_1 = s\sum_a \sum_{i,j,\sigma,\sigma'} \int d^2r \int d^2r' \Psi^\dagger_{i,\sigma}(r) \times U^{\sigma,\sigma'}_{a,i,j}(r,r')\Psi_{j,\sigma'}(r') , \quad (3)$$

where in the interaction potential centered on the a in-plane positions, we take into account the Coulomb scattering on nonmagnetic impurities U_0, and the exchange scattering on magnetic impurities U_1,

$$U^{\sigma,\sigma'}(p,p_z;q,q_z) = U_0(p,q)\delta_{\sigma,\sigma'} + \mathbf{S}\cdot\boldsymbol{\sigma} U_1(p,q) , \quad (4)$$

where $\mathbf{S}$ is the spin of the impurity atom in the magnetic case, and σ is the Pauli matrix. The scattering times τ_1 and τ_2 in the Born approximation are given by

$$\frac{1}{\tau_1} = \frac{nm}{2\pi s}\int_0^{2\pi} d\theta\, |U_0(\theta)|^2 ,$$
$$\frac{1}{\tau_2} = S(S+1)\frac{nm}{2\pi s}\int_0^{2\pi} d\theta\, |U_1(\theta)|^2 , \quad (5)$$

n being the concentration of the impurities on the unit area.

The renormalized gaps $\tilde{\Delta}$ and fermionic frequencies $\tilde{\omega}$ are given by

$$\tilde{\omega}_n = \omega_n + \frac{1}{2}\left(\frac{1}{\tau_1}+\frac{1}{\tau_2}\right)\tilde{\omega}_n F_0(\tilde{\omega}_n,\tilde{\Delta}) ,$$
$$\tilde{\Delta}_0 = \Delta_0 + \frac{1}{2}\left(\frac{1}{\tau_1}-\frac{1}{\tau_2}\right)[\tilde{\Delta}_0 F_0(\tilde{\omega}_n,\tilde{\Delta}) + \tilde{\Delta}_1 F_1(\tilde{\omega}_n,\tilde{\Delta})] , \quad (6)$$
$$\tilde{\Delta}_1 = \Delta_1, \quad \tilde{\Delta} = \tilde{\Delta}_0 + \tilde{\Delta}_1 \cos q_z s ,$$

and the gap equations become

$$\Delta_0 = -V_0\frac{m}{2\pi}\beta^{-1}\sum_n[\tilde{\Delta}_0 F_0(\tilde{\omega}_n,\tilde{\Delta}) + \tilde{\Delta}_1 F_1(\tilde{\omega}_n,\tilde{\Delta})] ,$$
$$\Delta_1 = -V_1\frac{m}{2\pi}\beta^{-1}\sum_n[\tilde{\Delta}_0 F_1(\tilde{\omega}_n,\tilde{\Delta}) + \tilde{\Delta}_1 F_2(\tilde{\omega}_n,\tilde{\Delta})] . \quad (7)$$

The kernel function is given by

$$F_i(\tilde{\omega}_n,\Delta) = \int_q \frac{\cos^i q_z s}{\tilde{\omega}_n^2 + \xi_q^2 + \tilde{\Delta}^2} ,$$
$$\int_q = \int d\varepsilon_q \int_{-\pi/s}^{\pi/s} \frac{dq_z}{2\pi} , \quad (8)$$

where $\xi_q = \varepsilon_q - \mu + J\cos q_z s$, and ε_q is the dispersion relation in two dimensions.

The possible solutions of the gap equations in the clean $n=0$ case were analyzed in Refs. 25 and 27. It was shown that away from half filling,[25] besides the simple superconducting phases ($\Delta_0 \neq 0$, $\Delta_1 = 0$ or $\Delta_0 = 0$, $\Delta_1 \neq 0$), a coexistence superconducting phase ($\Delta_0 \neq 0$, $\Delta_1 \neq 0$) with high T_c can appear within the system[27] taking into account a relatively small interlayer hopping J, and pairing V_1.[35] In the following, we present the in-plane impurity influence on the critical temperatures of the mentioned superconducting phases. The critical temperatures of the Δ_i simple superconducting phases, for $n=0$ ($n \neq 0$) is denoted by T_{i0} (T_i), $i=1,2$ and in the case of the coexistence superconducting phase by T_{c0} (T_c). The kernel function is expressed by taking into account a constant density of states for the two-dimensional dispersion, within the cutoff energy domain. If the density of states is picked in the vicinity of the Fermi surface, so its sharp can be modeled by a Dirac-δ-function behavior, and J is sufficiently small,[36] the deduced results remains quilitatively unchanged.

For $V_1=0$, only the in-plane phase exists ($\Delta_0 \neq 0$, $\Delta_1 = 0$), and the critical temperature T_0 for this case is given by

$$\mathcal{L}_0(T_0) = \ln\frac{T_0}{T_{00}} + \psi\left(\frac{1}{2}+\frac{1}{2\pi T_0 \tau_2}\right) - \psi(\tfrac{1}{2}) = 0 , \quad (9)$$

where $\psi(x)$ is the digamma function. As one can see, only the magnetic impurities act on this phase.

For a negligibly small J, F_1 vanishes for $\tilde{\Delta}_0 = 0$, so it is possible to obtain a pure interlayer phase: $\Delta_0 = 0$, $\tilde{\Delta}_1 \neq 0$, $\Delta_1 \neq 0$. In this case, the critical temperature T_1 is obtained from

$$\mathcal{L}_1(T_1) = \ln\frac{T_1}{T_{10}} + \psi\left[\frac{1}{2}+\frac{1}{4\pi T_1}\left(\frac{1}{\tau_1}+\frac{1}{\tau_2}\right)\right] - \psi(\tfrac{1}{2}) = 0 . \quad (10)$$

In this case, both magnetic and nonmagnetic impurities act on the superconducting phase. In fact, the influence of the nonmagnetic impurities on the interlayer pairing was claimed many years ago.[21] It was also underlined recently in a simple model which only considered the interaction between the electrons situated in neighboring layers through the exchange of three-dimensional phonons, but took into account free motion of the carriers inside each layer, and neglected the interlayer hopping.[23]

It is important to note here, that from Eq. (10), the $T_1 = T_1(1/\tau_1, 1/\tau_2)$ function, in the limit $n \to 0$, has identical slope $\partial T_1/\partial(1/\tau_i)$, for $i=1,2$. So the decrease, of the T_1 transition temperature as a function of the concentration, is made with the same slope at $n \to 0$ for both magnetic and nonmagnetic impurities.

For the coexistence superconducting phase $\Delta_0 \neq 0$, $\Delta_1 \neq 0$, the equation of the critical temperature has the form

$$\left[1 - |V_0|\pi T_c \frac{m}{2\pi}\sum_n \frac{F_0(\tilde{\omega}_n,0)}{1-\frac{1}{2}(1/\tau_1 - 1/\tau_2)F_0(\tilde{\omega}_n,0)}\right] \times \left[1 - |V_1|\pi T_c \frac{m}{2\pi}\sum_n \left[F_2(\tilde{\omega}_n,0) + \frac{\frac{1}{2}(1/\tau_1 - 1/\tau_2)F_1^2(\tilde{\omega}_n,0)}{1-\frac{1}{2}(1/\tau_1 - 1/\tau_2)F_0(\tilde{\omega}_n,0)}\right]\right] - 2\left[\frac{m}{2\pi}\Gamma\right]^2 = 0 , \quad (11)$$

where

$$\Gamma = \pi T_c \sum_n \frac{F_1(\tilde{\omega}_n,0)}{1-\frac{1}{2}(1/\tau_1 - 1/\tau_2)F_0(\tilde{\omega}_n,0)} . \tag{12}$$

For small impurity concentration, from Eq. (11) one gets

$$\left[\mathcal{L}_0(T_c)+\frac{A}{2}\left(\frac{1}{\tau_1}-\frac{1}{\tau_2}\right)\right]\left[\mathcal{L}_1(T_c)+\frac{B}{2}\left(\frac{1}{\tau_2}-\frac{1}{\tau_1}\right)\right]-2\Gamma^2+O\left[\left(\frac{J}{\Omega}\right)^2\right]=0 , \tag{13}$$

where

$$A=\pi T_c \sum_n F_0(\tilde{\omega}_n,0)F_1(\tilde{\omega}_n,0) , \quad B=\pi T_c \sum_n F_1^2(\tilde{\omega}_n,0) , \tag{14}$$

and Ω is the bandwidth.

Furthermore, we express $T_c = T_c(1/\tau_1, 1/\tau_2)$ at $n \rightarrow 0$ from Eq. (13), neglecting the $(J/\Omega)^2$ terms, obtaining

$$T_c + T_{c0} - K_1 \frac{1}{\tau_1} - K_2 \frac{1}{\tau_2} , \tag{15}$$

where

$$K_1 = \frac{(\pi/8)\ln(T_{c0}/T_{00}) + A(T_{c0}/2)\ln(T_{c0}/T_{10})}{2\ln[T_{c0}/(T_{00}T_{10})^{1/2}]} ,$$

$$K_2 = \frac{(\pi/8)\ln(T_{c0}/T_{00}) + (\pi/4)\ln(T_{c0}/T_{10}) - A(T_{c0}/2)\ln(T_{c0}/T_{10})}{2\ln[T_{c0}(T_{00}T_{10})^{1/2}]} . \tag{16}$$

As it can be seen from Eqs. (15) and (16), the slope of the $T_c = T_c(n)$ function at $n \rightarrow 0$ can be totally different for magnetic and nonmagnetic impurities. In the case $AT_{c0} > \pi/4$ (which usually is satisfied for $JT_{c0} > \Omega^2$), $K_1 > K_2$ can be obtained. It must be mentioned that $T_{c0} > T_{00}$ or T_{10} always[25,27] and $J=0$ implies $A \sim J = 0$. It is interesting to note that for $T_{c0} = T_{00}$ and $J=0$, we reobtain the classical AG result,[26] i.e., $K_1 = 0$ and $K_2 = \pi/4$. If J/Ω is close to unity, then we must take into account the neglected terms in Eq. (16) [starting from the $(J/\Omega)^2$ contribution]. In this case K_2 is substantially enhanced compared to K_1.

Finally, connected to these results, we make some remarks concerning the Zn doping in the 1:2:3 high-T_c materials. Zn is a divalent, nonmagnetic element, and its substitution for the in-plane Cu sites gives rise to a strong depression of the critical temperature.[37,38] This doping maintains both the orhtorhombicity (observed for other substitutions,[39] too) and the oxygen content of the lattice.[38,40] Starting from this experiment, Richert and Allen[41] performed a tight-binding calculation of the electronic structure of Zn-doped $YBa_2Cu_3O_{7-\delta}$, with d and s orbitals included for all the metal atoms, and p and s orbitals for the oxygen. Their results show that the Zn substitution gives rise only to minor changes in the valences and the density of states, which is, in contrast to the larger decrease in T_c, seen experimentally. They also claim that the direct electronic effect of Zn is small, and the shift in the Fermi energy and in the density of states at the Fermi energy is also weak. In such conditions, starting from the above presented model, it is possible to explain the observed T_c decrease caused by the Zn doping in the 1:2:3 material. This emphasizes once again the potential importance of the interlayer coupling, at least in the case of the 1:2:3 high-T_c materials.[42]

We must mention that a decrease in T_c given by nonmagnetic impurities can be deduced also for $V_1 = J = 0$, by taking into account only the anisotropic in-layer gap (see for example Ref. 22). But in this case $K_1 = K_2$, the the action of the magnetic impurities is strongly diminished compared to the AG result,[26] which clearly contradicts the experimental data.[15–19,37–40,42]

The authors kindly acknowledge the hospitality of the International Centre of Theoretical Physics, Trieste, where parts of this work were presented and discussed. The authors also wish to thank G. Baskaran, A. Bishop, D. C. Johnston, and A. Ruckenstein for stimulating discussions on high-T_c problems.

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