Interlayer pairing in layered superconductors

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A model of layered superconductors with exclusively interlayer pairing is studied. It is shown that singlet and triplet interlayer pairing have the same amplitude as long as the hopping between the layers is not too large and the effective interaction is dispersionless. However, a dispersion of the effective interaction results in the splitting of the critical temperature of singlet and triplet pairing for a finite hopping amplitude. It is shown that not only impurities in the layers but also impurities between the layers depress the critical temperature of interlayer pairing. Additionally, it is shown that impurities between the layers scattering electrons hopping from layer to layer lead to a stronger depression of triplet than of singlet interlayer pairing so that the critical temperature is split. We derive expressions for physical properties which are sensitive to the structure of the order parameter: the anisotropic penetration depth, the Josephson current to a conventional superconductor, the magnetic susceptibility which determines the Knight shift, and the jump in the specific heat in the case of the splitting of the transition temperature. We discuss experiments on layered high-temperature superconductors and conclude that the existence of interlayer pairing cannot be excluded in the superconducting state of these compounds.

I. INTRODUCTION

Since the discovery of high-temperature superconductivity[1] the interest in layered superconductors has risen drastically. A common feature of most of the layered high-temperature superconductors is the quasi-two-dimensionality of their electron system. Irrespective of which of all possible pairing mechanisms is responsible for high-temperature superconductivity, there is the possibility that not only electrons in one layer are bound to pairs but also electrons in weakly coupled neighboring layers. Layered superconductors have been studied both experimentally and theoretically, since the late 1960's.[2] The possibility of interlayer pairing with coexistence of singlet and triplet pairing has been already considered.[3] Nonmagnetic impurities suppress interlayer pairing, and it was believed not to exist in layered superconductors known at that time because these superconductors had a small mean free path compared with their coherence length.[4] Because of the high critical temperature of the new superconductors and their small coherence length $\xi \approx 10$ Å, which is smaller than their mean free path $l \approx 100$ Å,[5] a possible interlayer pairing would not be suppressed by small concentrations of nonmagnetic impurities.

There has been a series of articles recently that studied the possibility of interlayer pairing and also pointed out the influence of nonmagnetic impurities on T_c,[6–8] but disregarded the coexistence of singlet and triplet pairing. However, due to the separation of the electrons of one Cooper pair in neighboring layers the effective attractive interaction between them must necessarily be degenerated with respect to the spin of the electrons because the contribution of the exchange interaction remains small as long as the hopping amplitude between layers is small. Recently we learned that Klemm and Liu have studied the competition between *s*-wave intralayer pairing and interlayer pairing using the correct order parameter[9] but neglected some consequences of hopping between the layers.

In this article a model with purely interlayer pairing is studied in order to consider possible novel features of this unconventional type of pairing. We will not specify the mechanism of the attractive interaction between electrons in neighboring layers. A possible mechanism is the polarization of a dielectric spaced between the layers. This possibility was recently studied for layered high-temperature superconductors.[10,11] While it is known that the amplitudes of singlet and triplet pairing without hopping between the layers are equal,[3] we will show here that hopping can invalidate this equality and give rise to a splitting of the transition temperature if the interlayer interaction is dispersive in the momentum parallel to the layers. We would like to stress that this splitting of T_c has to be distinguished from the one obtained in Ref. 9, which is due to the dispersion of the effective interaction in the momentum perpendicular to the layers arising from the presence of more than one conducting layer per unit cell. Nonmagnetic impurities in the layers are known to depress the critical temperature of interlayer pairing, since they break the symmetry of the Cooper pairs.[4,12] Here we show that nonmagnetic impurities between the layers also give rise to a depression of T_c. Impurities that scatter electrons hopping from layer to layer are shown to cause a splitting of T_c, since they act on singlet and triplet interlayer pairs in a different way. This splitting can be stronger than the hopping-induced splitting mentioned above.

In studying physical properties of the interlayer pairing we concentrate on those observables that are sensitive to the structure of the order parameter and especially discuss those measurements that were cited as being evidence against any kind of triplet pairing in $YBa_2Cu_3O_{7-\delta}$.[13] We argue that the observed low-temperature behavior of the magnetic penetration depth, measurements of the Knight shift, as well as experiments that give Josephson coupling[20] with conventional superconductors, cannot exclude the possibility of the kind of interlayer pairing that we propose. Finally we treated the consequences of the splitting of T_c on the jump in the specific heat at the transitions. We find that there is a jump at both the transition temperature of the singlet as well as the triplet order parameter. Having obtained these results, we were informed that the authors of Ref. 9 also considered the consequences of the splitting of T_c on the density of states as well as the specific heat. While the origin of the splitting of T_c in Ref. 9 is different from the one obtained in our model, as was pointed out above, the consequences on the density of states and the specific heat are similar.[14]

In the next section we will introduce the model of interlayer pairing, derive the temperature Green's functions describing the superconducting state, and discuss the structure of the order parameter of interlayer pairing. In Sec. III, the Ginzburg-Landau equations are derived from the self-consistency equation for the order parameter, and their solution is discussed. In Sec. IV, we study the influence of nonmagnetic impurities on interlayer pairing in detail. In Sec. V, we derive expressions for physical properties of interlayer pairing. In Sec. VI, we discuss the possible existence of interlayer pairing in high-temperature superconductors and give our conclusions.

II. INTERLAYER PAIRING IN LAYERED SUPERCONDUCTORS

We consider a system of parallel planes and assume an attractive effective potential between electrons located in neighboring planes. We start from the total Hamiltonian of the system of electrons, which are allowed to move in the planes or to hop between the planes, feeling the effective interaction V_{ij}:

$$H=-\sum_{i,\alpha}\int d^2\rho\bar{\psi}(\boldsymbol{\rho})_{\alpha i}\frac{\nabla_\rho^2}{2m}\psi(\boldsymbol{\rho})_{\alpha i}-\sum_{i,\alpha}\int d^2\rho[\bar{\psi}(\boldsymbol{\rho})_{\alpha i}W\psi(\boldsymbol{\rho})_{\alpha,i+1}+\bar{\psi}(\boldsymbol{\rho})_{\alpha i}W\psi(\boldsymbol{\rho})_{\alpha,i-1}-2\bar{\psi}(\boldsymbol{\rho})_{\alpha i}W\psi(\boldsymbol{\rho})_{\alpha i}]$$
$$-\tfrac{1}{2}\sum_{ij}\sum_{\alpha\beta}\int d^2\rho\, d^2\rho' V_{\alpha\beta ij}(\boldsymbol{\rho}-\boldsymbol{\rho}')\bar{\psi}(\boldsymbol{\rho})_{\alpha i}\bar{\psi}(\boldsymbol{\rho}')_{\beta j}\psi(\boldsymbol{\rho}')_{\beta j}\psi(\boldsymbol{\rho})_{\alpha i}\ . \tag{2.1}$$

Here $\psi(\boldsymbol{\rho})_{\alpha i}$ is the field operator of an electron in layer i with spin α. $\boldsymbol{\rho}$ is the coordinate in the plane. The distance between layers d is set equal to 1. We also set $\hbar=c=k_B=1$. W is the hopping parameter between layers and m is the effective electron mass.

From the imaginary time Heisenberg equations using temperature Green's functions and its Fourier transforms, with respect to the inlayer coordinates $\boldsymbol{\rho}$, the layer indices i and the imaginary time τ, defined by

$$G_{ij}(\boldsymbol{\rho}_1,\boldsymbol{\rho}_2,\tau_1-\tau_2)=T\sum_{\omega_n}e^{-i\omega_n(\tau_1-\tau_2)}\int\frac{d\mathbf{p}}{(2\pi)^2}\int_0^{2\pi}\frac{dq}{2\pi}e^{i\mathbf{p}(\boldsymbol{\rho}_1-\boldsymbol{\rho}_2)}e^{i(i-j)q}G_q(\mathbf{p},\omega_n)\ , \tag{2.2}$$

and the anomalous Green's function F accordingly, where the fermionic Matsubara frequencies are $\omega_n=\pi T(2n+1)$, we get the Gor'kov equations, describing the interlayer pairing model

$$(i\omega_n-\bar{\xi})G_q(\mathbf{p};\omega_n)+\Delta_q F_q^+(\mathbf{p};\omega_n)=1\ , \tag{2.3a}$$

$$(i\omega_n+\bar{\xi})F_q^+(\mathbf{p};\omega_n)+\Delta_q^* G_q(\mathbf{p};\omega_n)=0\ . \tag{2.3b}$$

The energy dispersion $\bar{\xi}$ is given by $\bar{\xi}=\xi-2W\cos q$, where $\xi=p^2/(2m)-\mu$. The Fermi surface is defined by $\bar{\xi}=0$, which gives a corrugated cylinder. The order parameter must satisfy

$$\Delta_q^*(\mathbf{p},\epsilon_m)=T\sum_{\omega_n}\int\frac{d\bar{\mathbf{p}}'\,dq'}{(2\pi)^3}V(\mathbf{p}-\mathbf{p}',q-q',\epsilon_m-\omega_n)F_{q'}^+(\mathbf{p}',\omega_n)\ . \tag{2.4}$$

The effective interaction of interlayer pairing has the general form

$$V_q(\mathbf{k},\nu_n)=2\cos q V_0(\mathbf{k},q,\nu_n)\ , \tag{2.5}$$

where ν_n is a bosonic Matsubara frequency $\nu_n=2\pi Tn$. As a simple model we will take V_0 to be of the form

$$V_0(\mathbf{k},q,\nu_n)=V\omega_0(\mathbf{k},q)^2/(\omega_0(\mathbf{k},q)^2+\nu_n^2)\ ,$$

where $V>0$ for an attractive effective interaction. Usually, in BCS theory a dispersion of ω_0 is not essential and, for simplicity, one considers only a constant frequency $\omega_0(\mathbf{k})=\omega_0$. But in the case of interlayer pairing even small momentum dependence of the effective interaction can become important if the hopping amplitude between the layers is finite. To study this effect we will consider a small dispersion of the frequency in the momentum parallel to the layers, while we neglect the dispersion in the momentum perpendicular to the layers: $\omega_0(\mathbf{k})=\omega_0+\alpha\Omega(\mathbf{k})$ where $\alpha>0$ is a small parameter and the function $\Omega(\mathbf{k})$ is symmetric, $\Omega(\mathbf{k})=\Omega(-\mathbf{k})$ and periodic, $\Omega(\mathbf{k}+\mathbf{G})=\Omega(\mathbf{k})$, $\mathbf{G}$ being a reciprocal lattice vector.

Let us now consider the structure of the order parameter corresponding to interlayer pairing. Because of the spatial separation of the electrons of a Cooper pair, the Pauli principle is not important and the singlet pairing no longer has to be dominant as it must for conventional BCS superconductors. Rather we should start with a superposition of singlet and triplet pairing and then solve the Gor'kov equations to see if singlet and triplet pairing can coexist or if one of them is suppressed in the thermal equilibrium. As is known from the study of liquid He^3, the order parameter of a triplet state has, in general, a rich structure with orbital, spin, and gauge degrees of freedom.[15,16] Since the orbital degree of freedom is broken for interlayer pairing, the general form of the order parameter is

$$\Delta_q = 2e^{i\varphi}(a\sigma_y \cos q - ib\sigma\mathbf{n}\sigma_y \sin q) = \Delta_q^S + \Delta_q^T , \quad (2.6)$$

where a and b are real and $\mathbf{n}$ is a unit vector fixing the direction of the total spin of the pair in the spin space. Here we assumed that the phase φ, the singlet pairing amplitude a, the triplet pairing amplitude b, and $\mathbf{n}$ do not depend on the coordinates in the thermal equilibrium. From the Gor'kov equations (2.3) we now obtain the temperature Green's functions:

$$F_q^+(\mathbf{p},\omega_n) = \frac{\Delta_q^*}{\omega_n^2 + \bar{\xi}^2 + \Delta_q^* \Delta_q} ,$$
$$G_q(\mathbf{p},\omega_n) = -\frac{i\omega_n + \bar{\xi}}{\omega_n^2 + \bar{\xi}^2 + \Delta_q^* \Delta_q} , \quad (2.7)$$

where the order parameter Δ satisfies the equation

$$\Delta_q^* = T \sum_{\omega_n} \int \frac{d\mathbf{p}' dq'}{(2\pi)^3} V(\mathbf{p}-\mathbf{p}', \epsilon_m - \omega_n) \times 2\cos(q-q') F_{q'}^+(\mathbf{p}',\omega_n) . \quad (2.8)$$

In the absence of hopping between the layers we see, that Eqs. (2.7) and (2.8), giving the order parameter in the thermal equilibrium, can be satisfied if $\Delta_q^* \Delta_q$ does not depend on q. Noting that

$$\Delta_q^* \Delta_q = 4a^2 \cos^2 q + 4b^2 \sin^2 q ,$$

we thus find

$$a = b = \tfrac{1}{2}\Delta_0 , \quad (2.9)$$

where Δ_0 satisfies the standard BCS self-consistency equation. The solution, Eq. (2.9), can be shown to minimize the free energy,[3,9] so that without hopping between the layers the amplitudes of singlet and triplet pairing are equal.

However, with hopping, Eq. (2.9) is no longer a solution of Eqs. (2.7) and (2.8) due to the q' dependence of the electron energy $\bar{\xi}$. Although the deviation of the correct result from Eq. (2.9) is rather small for small tunneling amplitude W, the finiteness of this parameter can lead to new effects, in particular to splitting the transition temperature for singlet and triplet interlayer pairing. As long as this splitting is small it can be studied with the help of Ginzburg-Landau equations.

III. GINZBURG-LANDAU EQUATIONS WITH HOPPING BETWEEN LAYERS

Let us derive the Ginzburg-Landau equations using Eqs. (2.7) and (2.8). From these we will be able to determine the critical temperature T_c and the order parameter in thermal equilibrium. Assuming that the momentum dependence of the effective interaction is weak, we expand the effective interaction, Eq. (2.5), up to first order in α so that the self-consistency equation (2.8) becomes

$$\Delta_q^* = T \sum_{\omega_n} \frac{m}{(2\pi)^2} \int_0^{2\pi} dq' V \cos(q-q') \int_{-\epsilon_F}^{\infty} d\xi' \frac{\omega_0^2}{\omega_0^2 + (\omega_n - \epsilon_m)^2} F_{q'}^+(\xi',\omega_n)$$
$$+ T \sum_{\omega_n} \int \frac{d\mathbf{p}' dq'}{(2\pi)^3} 2V \cos(q-q') \frac{2\omega_0(\omega_n - \epsilon_m)^2}{[\omega_0^2 + (\omega_n - \epsilon_m)^2]^2} \alpha \Omega(\mathbf{p}'-\mathbf{p}) F_{q'}^+(\xi(\mathbf{p}'),\omega_n) . \quad (3.1)$$

Note that the first term does not depend on the hopping amplitude W, since one can set ϵ_F equal to ∞ in good approximation so that one can shift the integration variable from ξ' to $\bar{\xi}' = \xi' - 2W\cos q'$, thus eliminating the q' dependence totally. Therefore, if one would only consider the first term in Eq. (3.1) the solution, Eq. (2.9), would still hold for a finite hopping amplitude W. The second term, however, depends on W, since the q' dependence cannot be transformed away as in the first term because the function Ω depends on ξ' rather than on $\bar{\xi}'$ in our model. Note that, if one considers a more general model with an additional dispersion in the momentum perpendicular to the layers, which we have neglected for simplicity, the q' dependence still cannot be transformed away as long as the total momentum dispersion of the effective interaction does not have exactly the form $V_0(\bar{\xi} = \xi - 2W\cos q)$. Thus, the effect, obtained in the following for our simplified, model, is, in general, not changed qualitatively by an additional q dispersion, while its magnitude will be diminished accordingly. To study the effect of the second term, we expand the function F^+ in Eq. (3.1) in the hopping amplitude W to second order. For a solution near T_c we can expand Eq. (3.1) around $a,b=0$, which gives the Ginzburg-Landau equation,

$$\Delta_q^* \tau = -[3\Delta_q^{S*} + \Delta_q^{T*}] C W^2 + [\Delta_q^{S*}(3a^2+b^2) + \Delta_q^{T*}(a^2+3b^2)] B , \quad (3.2)$$

where $\Delta_q = \Delta_q^S + \Delta_q^T$ is related to the singlet and triplet pairing amplitudes a,b by Eq. (2.6), and $B = 7\zeta(3)/[8(\pi T_{c0})^2]$, where $\zeta(z)$ is the Riemann-zeta function and $\tau = (T_{c0} - T)/T_{c0}$, where $T_{c0} = 2\gamma/\pi\omega_0 \exp[-2\pi/(mV)]$. The magnitude of the W dependence of the Ginzburg-Landau equations is determined by the constant C:

$$C=T_{c0}\sum_{\omega_n}\int\frac{d\mathbf{p}'}{2\pi}\frac{(\omega_n-\epsilon_m)^2}{[(\omega_n-\epsilon_m)^2+\omega_0^2]^2}\frac{2\omega_0}{m}\alpha\Omega(\mathbf{p}'-\mathbf{p})\times\left[-\frac{2}{(\omega_n^2+\xi'^2)^2}+\frac{8\xi'^2}{(\omega_n^2+\xi'^2)^3}\right]. \quad (3.3)$$

Since only excitations near the Fermi surface are important, we can expand the function Ω around it by putting the external momentum $\mathbf{p}$ on the Fermi surface and varying the vector $\mathbf{p}'$ close to it:

$$\Omega(\mathbf{p}'-\mathbf{p})|_{|\mathbf{p}|=p_F}=\Omega^{(0)}(\varphi)+\Omega^{(1)}(\varphi)\xi'+\tfrac{1}{2}\Omega^{(2)}(\varphi)\xi'^2 , \quad (3.4)$$

where φ is the angle between $\mathbf{p}'$ and $\mathbf{p}$. Using this expansion of Ω, we can perform the integration over ξ'. Finally, performing the Matsubara summation, we find

$$C=\frac{2\pi\alpha}{\omega_0 m V}\int_0^{2\pi}\frac{d\varphi}{2\pi}\Omega^{(2)}(\varphi) . \quad (3.5)$$

Now, we can solve the Ginzburg-Landau equation (3.2).

For $C>0$ we find

$$a^2=b^2=0 \quad \text{for } T>T_a , \quad (3.6a)$$

$$a^2=\frac{\tau}{3B}+\frac{C}{B}W^2, b^2=0 \quad \text{for } T_a>T>T_b , \quad (3.6b)$$

$$a^2=\frac{\tau}{4B}+\frac{C}{B}W^2 \text{ and } b^2=\frac{\tau}{4B} \quad \text{for } T_b>T>0 , \quad (3.6c)$$

where

$$T_a=T_{c0}(1+3CW^2), T_b=T_{c0} . \quad (3.7)$$

Thus, for $C>0$ the hopping between the layers enhances the critical temperature of singlet pairing, while the critical temperature for triplet pairing stays at the value it has without hopping between the layers. Note that for $C>0$ the considered dispersion increases the strength of the effective interaction, which explains the increase of the upper critical temperature T_a. We see that in the temperature region between T_b and T_a only singlet pairing $a\neq 0$ exists, while below T_b singlet and triplet interlayer pairing coexist. The singlet and triplet amplitudes have no jumps but only kinks both at T_a and T_b so that both transitions are second order. The unusual structure of the order parameter qualitatively changes the density of states $N(\omega)$, which can be expressed in terms of the imaginary part of the Green's function, Eq. (2.7):

$$N(\omega)=-\int\frac{d\mathbf{p}\,dq}{(2\pi)^3}\,\mathrm{Im\,Tr}G_q(\mathbf{p},\omega_n)|_{i\omega_n\to\omega+i\eta} =\frac{2m}{\pi^2}\int_0^{\pi/2}dq\,\mathrm{Re}\frac{1}{[\omega^2-4b^2-4(a^2-b^2)\cos^2 q]^{1/2}} \quad (3.8)$$

Finally we get

$$N(\omega)=\frac{2m}{\pi^2}\omega\begin{cases}(\omega^2-4b^2)^{-1/2}K(L) & \text{for } \omega>2a ,\\ [4(a^2-b^2)]^{-1/2}K(L^{-1}) & \text{for } 2b<\omega<2a ,\\ 0 & \text{for } 0<\omega<2b ,\end{cases} \quad (3.9)$$

where K is the complete elliptic integral and

$$L=2[(a^2-b^2)/(\omega^2-4b^2)]^{-1/2} .$$

We see that in the region $T_b<T<T_a$ the order parameter has nodes, resulting in a gapless density of states with $N(\omega)\sim\omega$ as $\omega\to 0$ [see Fig. 1(a)]. For $T<T_b$ the gap in the density of states is diminished to $2b$ and there is no longer a singularity but a remarked peak at $\omega=2a$, instead [see Fig. 1b)].

For $C<0$ we find

$$a^2=b^2=0 \quad \text{for } T>T_b , \quad (3.10a)$$

$$a^2=0, b^2=\frac{\tau}{3B}+\frac{C}{3B}W^2 \quad \text{for } T_a<T<T_b , \quad (3.10b)$$

$$a^2=\frac{\tau}{4B}+\frac{C}{B}W^2 \text{ and } b^2=\frac{\tau}{4B} \quad \text{for } T<T_a , \quad (3.10c)$$

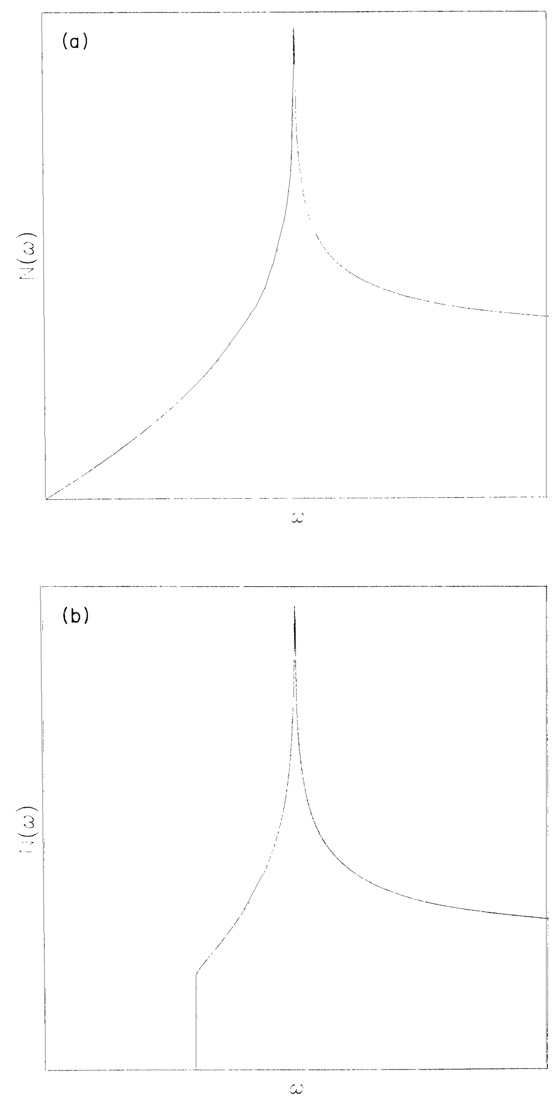

FIG. 1. (a) The gapless density of states in region where either singlet or triplet interlayer pairing exists, exclusively. (b) The density of states in region with coexistence of singlet and triplet interlayer pairing with unequal but nonzero amplitudes.

where

$$T_b = T_{c0}(1-|C|W^2), \quad T_a = T_{c0}(1-4|C|W^2) \; . \quad (3.11)$$

Thus, for $C<0$ the critical temperature of singlet is stronger diminished than that of triplet interlayer pairing and there is a temperature region, between T_a and T_b where there is only triplet interlayer pairing. The weakening of the strength of the effective interaction by the dispersion for $C<0$ explains the decrease of the upper critical temperature. Note that the singlet and triplet pairing amplitudes are continuous functions for any temperature and show kinks at both transitions. For $C<0$ the density of states is

$$N(\omega) = \frac{2m}{\pi^2}\omega \begin{cases} (\omega^2-4a^2)^{-1/2}K(L') & \text{for } \omega > 2b \; , \\ [4(b^2-a^2)]^{-1/2}K(L'^{-1}) & \text{for } 2b > \omega > 2a \; , \\ 0 & \text{for } 0<\omega<2b \; , \end{cases} \quad (3.12)$$

where

$$L' = 2[(b^2-a^2)/(\omega^2-4a^2)]^{-1/2} \; .$$

Here the density of states is gapless in the temperature region $T_a < T < T_b$ [see Fig. 1(a)]. For $0<T<T_a$ the gap is diminished to $2a$ and there is a remarked peak in the density of states at $\omega = 2b$ [see Fig. 1(b)].

The results of this section show that a finite hopping amplitude between the layers can result in a splitting of the transition temperature of interlayer pairing if there is dispersion of the effective interaction. For temperatures below the lowest transition singlet and triplet states coexist, whereas in the region between the two transitions only one of these states is possible, depending on the sign of the second derivative of the effective interaction, integrated over the Fermi surface. In the next section we show that splitting of the transition temperature can additionally be caused by scattering of the electrons from nonmagnetic impurities and that all kinds of nonmagnetic impurities lead to a depression of the transition temperature of interlayer pairing.

IV. INFLUENCE OF NONMAGNETIC IMPURITIES

The influence of nonmagnetic impurities on interlayer pairing is strongly dependent on the position of the impurities in the layered compound. Here, three cases are considered to which all other possibilities can be reduced: impurities in the conducting layers (I impurities), impurities between conducting layers scattering electrons that move in the planes (BI impurities), and impurities between conducting layers that scatter electrons from layer to layer (B impurities). Here, we indicated in parenthesis the abbreviations we will use below. We neglect any quantum corrections that are known to depress T_c additionally to the depression we derive here.[17]

At first we consider I impurities, which are expected to depress T_c, since they break the symmetry of interlayer paired Cooper pairs. To prove this we add the following impurity interaction to the total Hamiltonian:

$$H^{\mathrm{I}}_{\mathrm{imp}} = \int d\rho \sum_{\alpha,i,l} \rho_l J^I(\rho - \mathbf{R}_l)\delta_{r_l i}\bar{\psi}_{\alpha i}(\rho)\psi_{\alpha i}(\rho) \; . \quad (4.1)$$

Here it is summed over all I impurities l sitting at $(\mathbf{R}_l, r_l)$. ρ_l is a random variable, which is 1 if there is an impurity at $(\mathbf{R}_l, r_l)$ and 0 if there is none. J^{I} is the scattering potential of the I impurities. Since the impurities are randomly distributed, the system is not translationally invariant. Therefore, the Fourier transform of the Green's function is now defined as

$$G_{ij}(\rho_1,\rho_2,\tau_1-\tau_2) = T\sum_{\omega_n} e^{-i\omega_n(\tau_1-\tau_2)} \int \frac{d\mathbf{p}\, d\mathbf{p}'}{(2\pi)^4} e^{i\mathbf{p}\cdot\rho_1} e^{-i\mathbf{p}\cdot\rho_2} G_{ij}(\mathbf{p},\mathbf{p}';\omega_n) \; , \quad (4.2)$$

and the anomalous Green's function, accordingly. Using the same line of derivation as for Eqs. (3.2), but still using the representation of layer indices, we arrive at the Gor'kov equations in the presence of I impurities:

$$(i\omega_n - \xi - 2W)G_{ij}(\mathbf{p},\mathbf{p}';\omega_n) + W[G_{i-1,j}(\mathbf{p},\mathbf{p}';\omega_n) + G_{i+1,j}(\mathbf{p},\mathbf{p}';\omega_n)] + \int \frac{d\mathbf{p}''}{(2\pi)^2} \sum_l \rho_l J^I(\mathbf{p}-\mathbf{p}'')\delta_{r_l i} G_{ij}(\mathbf{p}'',\mathbf{p}';\omega_n) e^{i(\mathbf{p}-\mathbf{p}'')\cdot\mathbf{R}_l} + \Delta_{ik}F^{+}_{kj}(\mathbf{p},\mathbf{p}';\omega_n) = \delta_{ij}\delta(\mathbf{p}-\mathbf{p}') \; , \quad (4.3a)$$

$$(i\omega_n + \xi + 2W)F^{+}_{ij}(\mathbf{p},\mathbf{p}';\omega_n) - W[F^{+}_{i-1,j}(\mathbf{p},\mathbf{p}';\omega_n) + F^{+}_{i+1,j}(\mathbf{p},\mathbf{p}';\omega_n)] - \int \frac{d\mathbf{p}''}{(2\pi)^2} \sum_l \rho_l J^I(\mathbf{p}-\mathbf{p}'')\delta_{r_l i} F^{+}_{ij}(\mathbf{p}'',\mathbf{p}';\omega_n) e^{i(\mathbf{p}-\mathbf{p}'')\cdot\mathbf{R}_l} + \Delta^{*}_{ik}G_{kj}(\mathbf{p},\mathbf{p}';\omega_n) = 0 \; . \quad (4.3b)$$

Now, we average over I impurities, sitting in the layers. We follow the scheme by Abrikosov, Gor'kov, and Dzyaloshinski.[18] In the Born approximation it is sufficient to consider only diagrams that contain two scatterings from the same impurity, at the most. Furthermore, one can neglect all impurity-crossed diagrams, since they correspond to large momentum transfers, giving only a small contribution near the Fermi surface. Thus, we find that the impurity-averaged Green's functions are given by

$$G_{ij}(\mathbf{p};\omega_n) = G^0_{i-j}(\mathbf{p};\omega_n) + \begin{bmatrix} G^0_{i-k}(\mathbf{p};\omega_n) \\ F^0_{i-k}(\mathbf{p};\omega_n) \end{bmatrix}^T \begin{bmatrix} \bar{G}_{kl}(\omega_n) & -\bar{F}_{kl}(\omega_n) \\ -\bar{F}^{+}_{kl}(\omega_n) & -\bar{G}_{kl}(-\omega_n) \end{bmatrix} \begin{bmatrix} G_{lj}(\mathbf{p};\omega_n) \\ F^{+}_{lj}(\mathbf{p};\omega_n) \end{bmatrix} \; , \quad (4.4a)$$

$$F^+_{ij}(\mathbf{p};\omega_n)=F^{+0}_{i-j}(\mathbf{p};\omega_n)+\begin{bmatrix}G^0_{i-k}(\mathbf{p};-\omega_n)\\ F^{+0}_{i-k}(\mathbf{p};\omega_n)\end{bmatrix}^T\begin{bmatrix}\bar{F}^+_{kl}(\omega_n) & \bar{G}_{kl}(-\omega_n)\\ \bar{G}_{kl}(\omega_n) & -\bar{F}_{kl}(\omega_n)\end{bmatrix}\begin{bmatrix}G_{lj}(\mathbf{p};\omega_n)\\ F^+_{lj}(\mathbf{p};\omega_n)\end{bmatrix}, \tag{4.4b}$$

where

$$\bar{G}_{ij}(\omega_n)=n\int\frac{d\mathbf{p}''}{(2\pi)^2}|J^{\mathrm{I}}(\mathbf{p}-\mathbf{p}'')|^2\delta_{ij}G_{ij}(\mathbf{p}'';\omega_n), \tag{4.5a}$$

$$\bar{F}^+_{ij}(\omega_n)=n\int\frac{d\mathbf{p}''}{(2\pi)^2}|J^{\mathrm{I}}(\mathbf{p}-\mathbf{p}'')|^2\delta_{ij}F^+_{ij}(\mathbf{p}'';\omega_n). \tag{4.5b}$$

Here G^0 and F^0 are the Green's functions in the absence of impurities as given by Eq. (2.7). Transforming to momentum space perpendicular to the layers [compare with Eq. (2.2)], substituting Eq. (2.7) for G^0 and F^{+0}, and combining the above equations for the impurity averaged Green's functions, we arrive at the following equations:

$$\tilde{\Delta}^*_q G_q(\mathbf{p};\omega_n)+(i\tilde{\omega}_n+\xi)F^+_q(\mathbf{p};\omega_n)=0, \tag{4.6a}$$

$$(i\tilde{\omega}_n-\xi)G_q(\mathbf{p};\omega_n)+\tilde{\Delta}_q F^+_q(\mathbf{p};\omega_n)=1, \tag{4.6b}$$

where the frequency and the order parameter are renormalized due to the scattering by the I impurities as given by

$$i\tilde{\omega}_n=i\omega_n-\bar{G}_{\omega_n},\ \tilde{\Delta}^*_q=\Delta^*_q+\bar{F}^+_{\omega_n}, \tag{4.7}$$

where

$$\bar{G}_{\omega_n}=n\int\frac{d\mathbf{p}'\,dq'}{(2\pi)^3}|J(\mathbf{p}-\mathbf{p}')|^2G_{\omega_n}(\mathbf{p}',q'), \tag{4.8a}$$

$$\bar{F}^+_{\omega_n}=n\int\frac{d\mathbf{p}'\,dq'}{(2\pi)^3}|J(\mathbf{p}-\mathbf{p}')|^2F^+_{\omega_n}(\mathbf{p}',q'). \tag{4.8b}$$

For small impurity concentration n we can expand in the scattering rate

$$\frac{1}{\tau_{\mathrm{I}}}=\frac{nm}{2\pi}\int d\phi|J^{\mathrm{I}}(\phi)|^2, \tag{4.9}$$

where ϕ is the scattering angle in the planes. For the frequency renormalization (self-energy) we find thus to first order in the scattering rate

$$\bar{G}_{\omega_n}=-\frac{i}{2\tau_{\mathrm{I}}}\operatorname{sgn}(\omega_n). \tag{4.10}$$

The renormalization of the order parameter is, to first order in the scattering rate, given by

$$\bar{F}^+_{\omega_n}=\frac{1}{\tau_{\mathrm{I}}}\int_{-\epsilon_F}^{\infty}\frac{d\xi'}{2\pi}\times\int_0^{2\pi}\frac{dq'}{2\pi}\frac{\Delta^{S*}\cos q'+\Delta^{T*}\sin q'}{\omega_n^2+(\xi'-2W\cos q')^2+\Delta^*_{q'}\Delta_{q'}}, \tag{4.11}$$

where we made the q' dependence explicit by using

$$\Delta^*_q=\Delta^{S*}\cos q+\Delta^{T*}\sin q.$$

In the absence of the hopping between the layers the integral over the momentum perpendicular to the layers vanishes due to the specific structure of the interlayer pairing. For finite W, we can expand in W and find in the first order

$$\bar{F}^+_{\omega_n}=\Delta^{S*}\frac{W}{2\pi\tau_{\mathrm{I}}\epsilon_F^2}. \tag{4.12}$$

Thus, the renormalization of the effective attractive interlayer interaction by I impurities represented by $\bar{F}^+_{\omega_n}$ does vanish for triplet pairing and is negligible for singlet pairing as long as $W\ll\epsilon_F$. The physical reason is that for a small hopping amplitude the probability that both electrons of one interlayer paired Cooper pair are scattered from the same impurity is small. As a consequence, the vertex correction is small. This results in a depression of T_c since the renormalization of ω_n and Δ^* cannot be transformed away in the self-consistency equation as for nonmagnetic impurities in an isotropic superconductor. Solving the linearized self-consistency equation, using the obtained impurity-averaged anomalous Green's function, we find that the critical temperature T_c is depressed linearly with a scattering rate that is proportional to the concentration of nonmagnetic impurities in the planes, in agreement with Ref. 12:

$$T_c=T_{c0}-\frac{\pi}{8\tau_{\mathrm{I}}}. \tag{4.13}$$

We note that, if we do not neglect the small renormalization of the singlet order parameter, one finds that the critical temperature of singlet pairing is larger than that of triplet pairing. This splitting of T_c is of the order $(W\omega_0)/(\tau_{\mathrm{I}}\epsilon_F^2)$ which is much smaller than the splitting induced by scattering by B impurities, which is derived below.

Next we consider the influence of BI impurities sitting between the conducting layers, scattering electrons moving in the layers, as described by the Hamiltonian

$$H^{\mathrm{BI}}_{\mathrm{imp}}=\int d\rho\sum_{ail}\rho_l J^{\mathrm{BI}}(\rho-\mathbf{R}_l)\bar{\psi}_{ai}(\rho)\psi_{ai}(\rho)(\delta_{r_l i+1/2}+\delta_{r_l i-1/2}), \tag{4.14}$$

where the notation is as before and J^{BI} is the impurity scattering potential of the BI impurities, which is felt by the electrons moving in the planes. Deriving the Gor'kov equations, averaging over impurities as described above and transforming to momentum space with respect to the layer indices, we find that the BI impurities give the following renormalization of the frequency and the order parameter, respectively:

$$\bar{G}_{\omega_n}(q)=n\int\frac{d\mathbf{p}'dq'}{(2\pi)^3}|J^{\mathrm{BI}}(\mathbf{p}-\mathbf{p}')|^2 2[1-\cos(q-q')]G_{\omega_n}(\mathbf{p}',q') , \tag{4.15a}$$

$$\bar{F}^+_{\omega_n}(q)=n\int\frac{d\mathbf{p}'dq'}{(2\pi)^3}|J^{\mathrm{BI}}(\mathbf{p}-\mathbf{p}')|^2 2[1+\cos(q-q')]F^+_{\omega_n}(\mathbf{p}',q') . \tag{4.15b}$$

Expanding in the scattering rate

$$\frac{l}{\tau_{\mathrm{BI}}}=\frac{nm}{2\pi}\int d\phi|J^{\mathrm{BI}}(\phi)|^2 , \tag{4.16}$$

we find to first order

$$\bar{G}_{\omega_n}(q)=-\frac{i\,\mathrm{sgn}(\omega_n)}{\tau_{\mathrm{BI}}} , \quad \bar{F}^+_{\omega_n}(q)=\frac{\Delta^*_q}{2\tau_{\mathrm{BI}}|\omega_n|} . \tag{4.17}$$

Note that the self-energy correction $\bar{G}_{\omega_n}$ is twice the correction one would get from impurities with the same scattering strength, sitting in the layers. The reason is that an electron moving in the planes sees the BI impurities sitting both above and below its layer, so that it sees an impurity concentration $2n$ instead of n as for impurities in the planes. But the vertex correction represented here by $\bar{F}^+_{\omega_n}$ is caused by n impurities, only. This can be understood in the following way: the vertex corrections arise from the scattering of both electrons of an interlayer paired Cooper pair from the same BI impurity, which is only possible for the n BI impurities sitting between these two neighboring layers. Thus, the renormalization by the BI impurities cannot be transformed away in the self-consistency equation so that T_c is depressed. Solving the linearized self-consistency equation, we get a linear depression of T_c by BI impurities:

$$T_c=T_{c0}-\frac{\pi}{8\tau_{\mathrm{BI}}} , \tag{4.18}$$

Thus, the depression of T_c by BI impurities has exactly the same form as the depression by I impurities, Eq. (4.13). However, since the impurity potential decreases rapidly with distance, the scattering rate due to BI impurities τ_{BI} is expected to be small so that the depression of T_c by BI impurities is smaller than the one by I impurities as long as the concentration and strength of the BI impurities is not much larger than the one of the I impurities.

Finally, we study the influence of the B impurities sitting between the conducting layers and scattering only electrons hopping from layer to layer, as described by the Hamiltonian

$$H^{\mathrm{B}}_{\mathrm{imp}}=\int d\rho\sum_{\alpha il}\rho_l J^{\mathrm{B}}(\rho-\mathbf{R}_l)[\bar{\psi}_{\alpha i}(\rho)\psi_{\alpha,i-1}(\rho)\delta_{r_l i-1/2}+\bar{\psi}_{\alpha i}(\rho)\psi_{\alpha,i+1}(\rho)\delta_{r_l i+1/2}] , \tag{4.19}$$

where the notation is the same as before and J^{B} is the scattering potential of the B impurities. Deriving the Gor'kov equations, averaging over impurities as described above and going to momentum representation with respect to the layer indices we find that the renormalization by the B impurities is given by

$$\bar{G}_{\omega_n}(q)=n\int\frac{d\mathbf{p}'dq'}{(2\pi)^3}|J^{\mathrm{B}}(\mathbf{p}-\mathbf{p}')|^2 2[1+\cos(q+q')]G_{\omega_n}(\mathbf{p}',q') , \tag{4.20a}$$

$$\bar{F}^+_{\omega_n}(q)=n\int\frac{d\mathbf{p}'dq'}{(2\pi)^3}|J^{\mathrm{B}}(\mathbf{p}-\mathbf{p}')|^2 2]1+\cos(q+q')]F^+_{\omega_n}(\mathbf{p}',q') . \tag{4.20b}$$

It is important to note that the scattering potential appears here with a dependence on $q+q'$ rather than $q-q'$ as it does in the case of BI impurities. Consequently, the singlet and triplet order parameters enter with a different sign in the vertex correction. Expanding to first order in the scattering rate

$$\frac{1}{\tau_{\mathrm{B}}}=\frac{nm}{2\pi}\int d\phi|J^{\mathrm{B}}(\phi)|^2 , \tag{4.21}$$

we find that the self-energy correction is given by

$$\bar{G}_{\omega_n}=-i\frac{\mathrm{sgn}\omega_n}{\tau_{\mathrm{B}}} . \tag{4.22}$$

The renormalization of the order parameter is to the first order in the scattering rate given by

$$\bar{F}^+_{\omega_n}(q)=\frac{1}{\tau_{\mathrm{B}}}\int_{-\infty}^{\infty}\frac{d\xi'}{2\pi}\int_0^{2\pi}\frac{dq'}{2\pi}\frac{\Delta^{S*}\cos q\cos^2 q'-\Delta^{T*}\sin q\sin^2 q'}{\omega_n^2+(\xi'-2W\cos q')^2+\Delta^*_{q'}\Delta_{q'}} , \tag{4.23}$$

where we have neglected terms of order $(W\Delta^*)/(\tau_B \epsilon_F^2)$ by setting $\epsilon_F \to \infty$. Thus we find

$$\bar{F}^+_{\omega_n}(q) = \frac{1}{2\tau_B|\omega_n|}(\Delta_q^{S*} - \Delta_q^{T*}) . \tag{4.24}$$

The fact that the singlet and triplet order parameter enter with a different sign and prefactor in the vertex correction as represented by $\bar{F}^+$ results in a strong splitting of T_c as can be seen by deriving the Ginzburg-Landau equation analogous to Sec. III from the impurity renormalized self-consistency equation. We find

$$\tau\Delta_q^* = \Delta_q^{S*}\left[\frac{\pi}{8\tau_B T_{c0}} + B(3a^2+b^2)\right] + \Delta_q^{T*}\left[\frac{3\pi}{8\tau_B T_{c0}} + B(a^2+3b^2)\right] , \tag{4.25}$$

where τ is defined by $\tau = (T_{c0} - T)/T_{c0}$. The solution of this equation is given by

$$a^2 = b^2 = 0 \quad \text{for } T > T_a , \tag{4.26a}$$

$$a^2 = \frac{\tau}{3B} - \frac{\pi}{24\tau_B T_{c0} B} , \quad b^2 = 0 \quad \text{for } T_a > T > T_b , \tag{4.26b}$$

$$a^2 = \frac{\tau}{4B} , \quad b^2 = \frac{\tau}{4B} - \frac{\pi}{8B\tau_B T_{c0}} \quad \text{for } T_b > T , \tag{4.26c}$$

where $T_a > T_b$ are the transition temperatures for the singlet and triplet interlayer pairing, respectively, which are given by

$$T_a = T_{c0} - \frac{\pi}{8\tau_B} , \quad T_b = T_{c0} - \frac{\pi}{2\tau_B} . \tag{4.27}$$

Thus, the BI impurities, sitting between the layers, scattering electrons from layer to layer, cause a large splitting of the superconducting transition temperature, given by $\Delta T_c = 3\pi/8\tau_B$. Note that the singlet and triplet interlayer pairing amplitudes are continuous functions for any temperature and have only kinks at both transitions.

In this section, we found that scatterings of the electrons at nonmagnetic impurities in the layers as well as between the layers depress the transition temperature of the superconducting state with purely interlayer pairing. However, impurity scatterings from plane to plane more strongly suppress triplet pairing and therefore lead to a splitting of the transition temperature.

V. SOME PHYSICAL PROPERTIES

In this section we will study how some physical properties of layered compounds are influenced by interlayer pairing. We will concentrate on those observables that are sensitive to the structure of the order parameter: low-temperature behavior of the penetration depth, Josephson coupling with a conventional superconductor, Knight shift, and specific-heat jump at T_c.

Let us start with the response to a static magnetic field. It is well known that unconventional order parameters can lead to a power-law behavior of the magnetic penetration depth at low temperatures rather than a BCS-type exponential decay with temperature. However, by looking at the density of states of the system with purely interlayer pairing, as given by Eq. (3.9), which has a gap at low temperatures, one can guess that the penetration depth will have a BCS-type exponential behavior for $T \to 0$. To show this explicitly, we derive the current induced by the magnetic field $\mathbf{H} = \nabla \times \mathbf{A}$ in the linear response approximation. In the momentum representation the current components can now be written as

$$j_k(\mathbf{k},q) = -\frac{ne^2}{m_k} A_k(\mathbf{k},q) - P_{kl}(\mathbf{k},q,\omega=0) A_l(\mathbf{k},q) , \tag{5.1}$$

where $k,l \in [1,2,3]$, $m_1 = m_2 = m$, $m_3 = 1/(2W)$, and $P_{kl}(\mathbf{p},q,i\nu_n \to \omega + i\eta)$ is defined as the Fourier transform of the current-current correlation function in imaginary time, which is defined as

$$P_{kl}(\rho - \rho', i-j, \tau - \tau') = -\langle T_\tau [j_k^0(\rho,i,\tau) j_l^0(\rho',j,\tau)] \rangle , \tag{5.2}$$

where j^0 is the current operator without external field

$$j_k^0(\rho,i,\tau) = \frac{ie}{2m_k}(\nabla_1 - \nabla_2)|_{1\to 2}[\bar{\psi}(\rho_1,i_1,\tau)\psi(\rho_2,i_2,\tau)]|_{\rho_2=\rho,i_2=i} . \tag{5.3}$$

Note, that because of the discreteness in the direction perpendicular to the layers, the gradient component in this direction is defined to take the difference between the value of the function in neighboring layers:

$$(\nabla)_3 G(\rho,i,\tau) = G(\rho,i+1,\tau) - G(\rho,i,\tau) .$$

Applying Wick's theorem and noting that the expectation value of the current without magnetic field vanishes, we can write the current-current correlation function in terms of Green's functions:[19]

$$P_{kl}(\rho-\rho', i-j, \tau-\tau') = \frac{e^2}{4m_k m_l}(\nabla_1 - \nabla_2)_k (\nabla_3 - \nabla_4)_l |_{1\to 2, 3\to 4}[-G^0(1,4)G^0(3,2) + F^0(1,3)F^{+0}(4,2)] . \tag{5.4}$$

It is convenient to go now to the momentum representation, using

$$P_{kl}(\rho-\rho', i-j, \tau-\tau') = \int \frac{d\mathbf{p}\, dq}{(2\pi)^3} e^{i\mathbf{p}\cdot(\rho-\rho')} e^{iq(i-j)} T \sum_{\nu_n} e^{-i\nu_n(\tau-\tau')} P_{kl}(\mathbf{p},q,\nu_n) , \tag{5.5}$$

where $\nu_n = 2\pi T n$ are the bosonic Matsubara frequencies. Substituting Eq. (2.7) for the Green's functions in momentum space, we find

$$P_{kl}(\mathbf{k}\to 0, q\to 0, \omega=0) = -\frac{e^2}{2m_k^2}\int \frac{d\mathbf{p}\,dq'}{(2\pi)^3}\begin{bmatrix} 4p_k p_l & \text{for } k,l=1,2 \\ 4\sin^2 q' & \text{for } k=l=3 \\ 0 & \text{otherwise}\end{bmatrix}\frac{1}{4T}\cosh^{-2}\frac{E}{2T}\ , \tag{5.6}$$

where $E=(\xi^2+\Delta_{q'}\Delta^*_{q'})^{1/2}$ and we made an analytic continuation to the real frequency axis. Since we are interested in the response to static magnetic fields, we set the frequency $\omega=0$. Furthermore, we consider only the limit $\mathbf{k},q\to 0$, since most known layered superconductors are in the local (London) limit, which means that they have a small coherence length compared to their penetration depth. The current components can now be written as

$$j_k(\mathbf{k},q) = -\frac{n_k^S e^2}{m_k c}A_k(\mathbf{k},q)\ , \tag{5.7}$$

where n_k^S are the diagonal components of the anisotropic density tensor of superconducting electrons:

$$n_k^S = n - \frac{1}{8Tm_k}\int \frac{dp\,dq}{(2\pi)^2}p\begin{bmatrix} 2p^2 & \text{for } k=1,2 \\ 4\sin q^2 & \text{for } k=3\end{bmatrix}\cosh^{-2}\frac{E}{2T}\ . \tag{5.8}$$

Here, n is the density of electrons. Thus, we find that the low-temperature behavior of the penetration depth λ is given by

$$\frac{\lambda_k(T)}{\lambda_k(0)} - 1 = \frac{m}{4n}\epsilon_F\sqrt{b/\pi T}\left[1+\frac{a^2-b^2}{16b^2}\left[1-\frac{4b}{T}\right]\right]\exp\left[-\frac{2b}{T}\right]\begin{cases} W & \text{for } k=1,2 \\ \epsilon_{F_2} & \text{for } k=3\end{cases} \tag{5.9}$$

with

$$\lambda_3(0) = \frac{1}{e}\sqrt{m/4\pi n}\ , \quad \lambda_{1,2}(0) = \frac{1}{e}\sqrt{1/8\pi n W}\ . \tag{5.10}$$

Thus, even if the amplitudes of singlet and triplet interlayer pairing are unequal, $a\neq b$, the penetration depth decays exponentially as $T\to 0$ and the statement that triplet pairing is in disagreement with an exponential decay of the penetration depth at low temperatures[13] does not apply to the interlayer pairing under consideration.

Now, we will give an expression for the Josephson current between a conventional BCS superconductor and the layered compound with interlayer pairing only. The supercurrent between these two superconductors can be written in terms of the one-particle Green's function in the superconducting state, given by

$$G^S_{\omega_n}(\mathbf{r},\mathbf{r}') - G^N_{\omega_n}(\mathbf{r},\mathbf{r}') - \int ds\int ds' G^N_{\omega_n}(\mathbf{r},\mathbf{s})\Delta(\mathbf{s})G^N_{-\omega_n}(\mathbf{s}',\mathbf{s})\Delta^*(\mathbf{s}')G^S_{\omega_n}(\mathbf{s}',\mathbf{r}')\ . \tag{5.11}$$

Here, G^N is the Green's function in the normal state, defined by

$$\left[i\omega_n + \frac{1}{2m}\nabla_{\mathbf{r}}^2 + \mu\right]G^N_{\omega_n}(\mathbf{r},\mathbf{r}') = \delta(\mathbf{r}-\mathbf{r}')\ , \tag{5.12}$$

where ∇_3 is the continuous derivative for $\mathbf{r}\in V_1$, where V_1 is the volume of the conventional superconductor, whereas it is defined to take the difference of the function in neighboring layers if $\mathbf{r}\in V_2$, where V_2 is the volume of the layered superconductor. The order parameter $\Delta(\mathbf{r})$ is a complex constant $\Delta_1 e^{i\phi_1}$ if $\mathbf{r}\in V_1$, while it is defined by Eq. (2.6) if $\mathbf{r}\in V_2$. Following the derivation by Josephson,[20] we arrive at the following expression for the supercurrent:

$$I = 2ie\,\mathrm{Tr}T\sum_{\omega_n}\left[\int_{s'\in V_1}ds'\int_{s\in V_2}ds - \int_{s'\in V_2}ds'\int_{s\in V_1}ds\right]G^S_{-\omega_n}(\mathbf{s},\mathbf{s}')G^N_{\omega_n}(\mathbf{s}',\mathbf{s})\Delta(\mathbf{s})\Delta^*(\mathbf{s}')\ , \tag{5.13}$$

where the trace is taken over the spin. Near T_C we can substitute G^S by G^N and we find

$$I = \mathrm{Tr}\sum_{s=\pm 1}[K(\Delta_I a i\sin(\phi_1-\varphi) + \Delta_1 b\cos(\phi_1-\varphi)\sigma n s)]\ , \tag{5.14}$$

where

$$K = 2ieT\sum_{\omega_n}\int_{s'\in V_1}ds'\int_{s\in V_2}ds\, G^N_{-\omega_n}(\mathbf{s},\mathbf{s}')G^N_{\omega_n}(\mathbf{s}',\mathbf{s})\ . \tag{5.15}$$

Calculating the trace in Eq. (5.14) we find

$$I = 4K\Delta_1 a\sin(\phi_1-\varphi)\ , \tag{5.16}$$

Thus, only the singlet part of the interlayer order parameter contributes to the Josephson current. In the region of temperatures where the singlet pairing amplitude does not vanish, the Josephson current is not equal to zero, and its magnitude depends on the orientation of the layered compound to the interface with the conventional superconductor. For small hopping amplitude W, we have seen in Secs. II and III that $2a\approx 2b=\Delta_0$, where Δ_0 is defined by the standard BCS self-consistency equation, and we see that the supercurrent between a conventional and the layered superconductor with purely interlayer pairing is only half of the supercurrent one would get if one substituted the layered compound with another conventional superconductor with the order parameter Δ_0. Therefore, we conclude that the mere detection of a Josephson current, in principle, is not in disagreement with the mixed singlet and triplet pairing we proposed. Only if one could measure the magnitude of the Josephson current accurately and also know the amplitude of the order parameter from an independent measurement, definite conclusions about the existence of interlayer pairing could be drawn.

Now we derive the magnetic susceptibility, which determines the Knight shift. In terms of the Green's function, the spin susceptibility can be written as

$$\chi_{kl} = \left.\frac{\partial S_l}{\partial H_k}\right|_{H=0} = T\sum_{\omega_n}\int \frac{d\mathbf{p}\,dq}{(2\pi)^3}\,\mathrm{Tr}\sigma_l \frac{\partial}{\partial H_k} G_{\omega_n}(\mathbf{p},q)|_{H=0} , \tag{5.17}$$

where $k,l \in 1,2,3$. The Green's function G, which includes the paramagnetic interaction of the conducting electrons with the external magnetic field $\mathbf{H}$ is obtained from Eqs. (2.3) by substituting for $\xi - \sigma\mathbf{H}\,\xi$. Here, σ is the vector operator composed of the three Pauli matrices. Calculating the Matsubara frequencies and using the commutation relations for the Pauli matrices, we find

$$\chi_{ij} = \frac{m}{\pi}\left[\delta_{ij}Y + \frac{b}{a+b}(\delta_{ij} - n_i n_j)(1-Y)\right] , \tag{5.18}$$

where

$$Y = \int_0^\infty d\xi \frac{1}{2T}\frac{1}{\cosh^2(E/2T)} \tag{5.19}$$

is the Yossida function that has the properties $Y(T=0)=0$ and $Y(T=T_C)=1$ where we used, at low temperatures, $a \approx b$ so that the energy E in the integrand of the Yossida function is independent of the momentum perpendicular to the layers q in good approximation: $E \approx (\xi^2 + 4a^2)^{1/2}$. The magnetic field tends to orient the spin axis so as to minimize the magnetic free energy:

$$F_{\mathrm{magn}} = -\tfrac{1}{2}\chi_{ij}H_i H_j . \tag{5.20}$$

By substituting the expression for the susceptibility we find $\mathbf{Hn}=0$, which means that the spin axis is oriented along the magnetic field, since $\mathbf{n}$ is directed along the axis with vanishing spin projection as shown by Leggett.[15] This gives for the susceptibility in thermal equilibrium

$$\chi = \chi_n \left[Y + \frac{b}{a+b}(1-Y)\right] , \tag{5.21}$$

where $\chi_n = m/\pi$ is the susceptibility of the normal state. Thus, the Knight shift $K^s \propto \chi$ is nonvanishing at $T=0$ as long as the triplet pair amplitude $b(T=0) \neq 0$:

$$\chi(T=0) = \chi_n \frac{b}{a+b} . \tag{5.22}$$

If the singlet and triplet pairing are equal at $T=0$ as is probable in view of the results obtained in Secs. II, III, and IV, the Knight shift at $T=0$ is half of the Knight shift in the normal state.

Finally, we study the effect of splitting of T_c on the specific heat. The jump of the specific heat at a superconducting transition is given by[16]

$$\Delta C_V = -\frac{1}{2}N(0)\frac{\partial}{\partial T}\mathrm{Tr}(\Delta^*\Delta) = -2N(0)\frac{\partial}{\partial T}(a^2+b^2) , \tag{5.23}$$

where we used the order parameter of interlayer pairing, Eq. (2.6). At the higher transition temperature we find, using Eqs. (3.6b), (3.10b), and (4.26b) for the respective jump in the specific heat, to lowest order,

$$\Delta C_V(T_a) = \frac{2N(0)}{3BT_c} , \tag{5.24}$$

while the jump in the specific heat at the transition to the coexistence phase is given to lowest order by

$$\Delta C_V(T_b) = \frac{N(0)}{3BT_c} , \tag{5.25}$$

where we used Eqs. (3.6c), (3.10c), and (4.26c), respectively. We note that for an experimental observation these two jumps must be well separated, which is only possible if the splitting of the transition temperature is large enough and the sample is homogeneous so that the transition temperatures in different regions of the sample do not differ much.

VI. DO EXPERIMENTS ON LAYERED HIGH-TEMPERATURE SUPERCONDUCTORS EXCLUDE INTERLAYER PAIRING IN THESE COMPOUNDS?

Numerous excellent experiments on almost all measurable observables of $YBa_2Cu_3O_{7-\delta}$ have been done since the discovery of superconductivity in this compound five years ago. Unfortunately, the set of experiments on other layered compounds is not yet complete so that we mainly have to restrict our discussion of the possible existence of interlayer pairing on $YBa_2Cu_3O_{7-\delta}$. For this compound, however, it is possible to give strong constraints on the possible structure of the order parameter of the superconducting state. However, while these constraints are strong enough to exclude a purely triplet paired state in this compound,[13] we want to point out now that they do not exclude the possibility of interlayer pairing, since in this case the triplet pairing is in coexistence with the singlet pairing in a large region of temperature as was shown in Secs. II and III.

The low-temperature behavior of the magnetic penetration depth of $YBa_2Cu_3O_{7-\delta}$ shows an exponential decay with temperature to a nonzero value at $T=0$.[13] Interlayer pairing shows this behavior as long as the splitting of T_c is not extremely large. The detection of persistent currents in superconducting rings consisting of part lead and part $YBa_2Cu_3O_{7-\delta}$ was interpreted as being evidence of pure singlet pairing, since lead is known to be a conventional singlet superconductor. As we have shown in the preceding section, the mere detection of a persistent current in such a system does not exclude the possibility of interlayer pairing. Particularly, interlayer pairing does not result in a depression of T_c of the mixed ring as long as the critical temperature of singlet interlayer pairing is close to that of triplet interlayer pairing. Only by the application of a high magnetic field parallel to the layers could one favor triplet interlayer pairing[3] and strongly depress T_c of singlet pairing so that the critical temperature for existence of a persistent current in the mixed ring would also be depressed if interlayer pairing exists. Unfortunately, the measurements known to us cannot give such information, since they present only data to prove that there is no measurable suppression of T_c in the mixed ring compared with the pure lead ring without the application of a strong magnetic field.[21]

The strongest evidence against pure triplet pairing in $YBa_2Cu_3O_{7-\delta}$ is given by measurements of the anisotropic Knight shift.[22] The consistent explanation of a large number of NMR experiments by a phenomenological theory,[23,24,13] which gives a vanishing Knight shift at $T=0$ after subtraction of the chemical shift using an estimation of its anisotropy, seems to rule out the existence of interlayer pairing in this compound, since it gives at $T=0$ a Knight shift of half of its normal value. But we note that there is some uncertainty in the estimation of the chemical shift anisotropy, since the electronic eigenfunctions in the CuO_2 layers are still a matter of controversy. This still leaves the possibility that there is a small nonvanishing Knight shift $K(T=0)$. Thus, we can conclude that the Knight-shift data of $YBa_2Cu_3O_{7-\delta}$ exclude the possibility of purely interlayer pairing, while its coexistence with intralayer pairing cannot be excluded in this compound. Additionally, the influence of spin-orbit coupling on the layered high-temperature superconductors still must be studied in detail. As was shown in Ref. 25, spin-orbit interactions in layered superconductors can give rise to modifications of the anisotropic susceptibility in the superconducting state where only intralayer pairing was considered. The influence of spin-orbit interactions on interlayer pairing will therefore be the subject of further study.

We note that the experimentally seen depression of T_c by nonmagnetic impurities as, for example, by the substitution of Cu atoms in $YBa_2Cu_3O_{7-\delta}$ by diamagnetic Zn ions[26] would have a natural explanation if there exists interlayer pairing in these compounds. Let us now estimate the upper bound for the splitting of T_c in $YBa_2Cu_3O_{7-\delta}$, which has a maximum T_c of 90 K. In $YBa_2Cu_3O_{7-\delta}$ the hopping amplitude between layers is approximately $W \approx 100$ K as obtained experimentally from the anisotropy of the lower and upper critical magnetic field[27] and theoretically from band-structure calculations.[28] The main part of the Fermi surface is known both by band theory and experiment to have a shape of a corrugated cylinder with $\epsilon_F \approx 1500$ K.[28] The cutoff parameter ω_0 and the strength of the dispersion depends on the pairing mechanism. As an example, we consider a phonon mediated effective attraction. The phonon dispersion curves of $YBa_2Cu_3O_{7-\delta}$ were calculated in Ref. 29. A typical optical phonon frequency is about 100 K. The dispersion amplitudes α range from 2 to 30 K depending on the respective phonon branch. Using $p_F \approx 2.8/a$, where a is the in-plane lattice constant,[28] we can calculate the constant C defined in Eq. (3.5), where we take

$$\Omega(\mathbf{p}-\mathbf{p}') \sim \cos(a|\mathbf{p}-\mathbf{p}'|)$$

as a typical phonon dispersion curve. Thus, we find as an upper bound for the hopping induced splitting of the critical temperature:

$$\Delta T \leq \alpha W^2/(\omega_0 \epsilon_F^2) T_{c0} \approx 0.1 \text{ K} .$$

Therefore, if the effective interaction is phonon mediated, this splitting of T_c is so small that it is not likely to be detected in any experiment on $YBa_2Cu_3O_{7-\delta}$. For the splitting of the critical temperature by nonmagnetic impurities in $YBa_2Cu_3O_{7-\delta}$, we can give an upper bound, using as a lower bound for the mean free path due to scattering from layer to layer by nonmagnetic impurities between the layers $l \approx 100$ Å, which is known to be the total average mean free path, mainly due to scatterings at impurities in the layers.[5] Thus, we find the scattering rate to be at the most $1/\tau \leq 1.1 \times 10^{12}$ /sec^{-1} so that the splitting of T_c has the upper bound $\Delta T_c = 3/(8\tau) \approx 30$ K. We see that the splitting by impurities could be considerably larger than the hopping-induced splitting of the transition temperature. However, the actual mean free path corresponding to scattering from plane to plane by impurities between the layers should be much larger than the total mean free path taken as a lower bound. Therefore, the splitting is probably so small that it will not lead to measurable effects such as the appearance of a double peak in the specific heat, since this can only be seen for a large splitting of T_c, because spatial inhomogeneity smears out the lower peak if the peaks are close to each other. The specific heat of $YBa_2Cu_3O_{7-\delta}$ near T_c is one of the most extensively studied thermal properties. The huge majority of experiments see only one jump in the specific heat[30] and the exceptions[31] can be explained by the inhomogeneities of the samples as done by a theory of Abrikosov.[32] Thus, we can conclude that specific-heat measurements of $YBa_2Cu_3O_{7-\delta}$ exclude a large splitting of T_c in agreement with the results obtained above for a possible interlayer pairing.

In conclusion, it was shown that interlayer pairing results in some qualitatively new features such as the splitting of T_c by hopping between adjacent layers and by scattering from impurities between the layers. Not only nonmagnetic impurities in the layers, but also those between the layers, lead to a depression of the critical temperature of interlayer pairing. Our investigation of physical properties of interlayer pairing leads us to the conclusion that according to the present experimental situation on $YBa_2Cu_3O_{7-\delta}$, only the Knight-shift data indicate that the interlayer pairing plays a minor role in comparison to intralayer singlet pairing. However, in order to give a certain conclusion about the existence of interlayer pairing in layered high-temperature superconductors, it is necessary to have zero-temperature Knight-shift data of other layered superconductors, especially of those with a higher transition temperature such as $Tl_2Ba_2Ca_2Cu_3O_{10+\delta}$ and $Bi_2Sr_2CaCu_2O_{8+\delta}$, which are known to have a much larger mass anisotropy than $YBa_2Cu_3O_{7-\delta}$.[33,34] giving values for the hopping amplitude W smaller than 1 K so that the existence of interlayer pairing in these compounds is more likely. Therefore, it is worthwhile to extend our simple model to include intralayer pairing as was already done without triplet pairing[8] and recently for the correct order parameter including triplet pairing.[9] Furthermore, spin-orbit coupling and spin fluctuations could lead to modifications of our results and will be the subject of further work.

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