Spin-orbit scattering in dirty superconductors

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Spin-orbit scattering and the resulting spin contamination of the pure spin-up and spin-down states of a singlet Cooper pair lead to a finite *exchange* term in the pairing interaction, besides the *direct* term of BCS theory. Both of these terms are evaluated as functions of the spin lifetime τ_{so} and the effective coherence length ξ of a dirty superconductor. We show that, as τ_{so} decreases, the weakening of the direct term caused by spin rotation of the pair within ξ is exactly compensated by intervention of the exchange term. Both effects are proportional to $\xi/v_F\tau_{so}$ (where v_F is the Fermi velocity). The physical conclusion is that the transition temperature T_c remains unaffected, a result first noted by Anderson.

The theory of dirty superconductors[1] is based on the BCS interaction, I, that occurs between pairs of one-electron states which are exact time-reverse partners of each other. For ordinary impurity scattering, these scattered states are either pure spin-up or spin-down states. An impurity-induced change of the transition temperature, δT_c, can arise from anisotropy and band-structure effects.[2] The first effect is caused by a reduction of the (favorable) gap anisotropy. The resulting decrease in T_c saturates when the mean free path l is reduced to a value comparable to the coherence distance of the host, ξ_0.

Besides momentum scattering there can be spin-orbit (so) scattering by the impurities. In a macroscopic crystal, this scattering leads to complete spin contamination of a scattered state. Such states have no average spin component in any direction, as pointed out by Anderson[3] in the context of residual Knight shifts in superconductors. Consider the interaction I of the gap equation; all that matters is the spin rotation of an electron that occurs within the effective coherence length of a Cooper pair, $\xi=(\xi_0 l)^{1/2}$. This spin contamination (during the time that the electron needs to traverse ξ) introduces an exchange contribution to I, *absent* in BCS theory.

Why, then, does so scattering have no effect on T_c? The standard observation is that the time-reversal symmetry operator commutes with the so coupling operator. As a consequence there are still exact time-reverse partners from which to construct bound Cooper pairs. However, the off-diagonal matrix elements of the phonon-mediated interaction, which occur in the BCS integral equation, are altered in detail. As we show below, the direct matrix elements are reduced in magnitude, and new exchange terms arise. However, we subsequently find by explicit calculation that the two changes cancel.

We shall consider a host superconductor without so interaction, but we assume that the scattering potentials of the impurity atoms contain significant so coupling. Then, the interaction terms of the gap equation involve both direct (dir) and exchange (ex) contributions between time-reversed pairs, cf. Fig. 1. What matters for the interaction in the linear-gap equation at T_c is the degree of spin rotation within the effective coherence distance ξ. The wave functions for the two partners of a time-reversed pair are written as

$$\psi_n=\phi_n\left[\alpha\cos\frac{\theta}{2}+\beta e^{i\phi/2}\sin\frac{\theta}{2}\right], \quad (1)$$

$$\psi_{\bar n}=\phi_n^*\left[\beta\cos\frac{\theta}{2}-\alpha e^{-i\phi/2}\sin\frac{\theta}{2}\right]. \quad (2)$$

Here $\phi_n=\sum_{\vec k}(n\mid\vec k)\psi_{\vec k}$ solves the impurity scattering problem in the absence of so scattering, $\psi_{\vec k}$ are Bloch functions, and α,β are the spin eigenfunctions of σ_z. The spin rotation away from the z axis is measured by the angles θ,ϕ. It must be emphasized that θ and ϕ generally depend on n, and are slowly varying functions of $\vec r$. We neglect this latter dependence since the length scale is $v_F\tau_{so}$ where τ_{so} is the spin lifetime. With the basis functions defined by (1) and (2), the interaction in the T_c equation is given by

$$I_{nn'}=I^{\rm dir}(n\to n',\ \bar n\to\bar n')-I^{\rm ex}(n\to\bar n',\ \bar n\to n'), \quad (3)$$

where

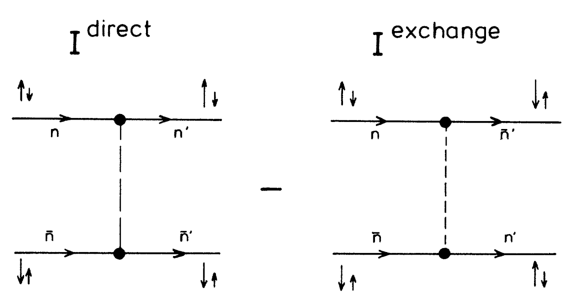

FIG. 1. Direct and exchange contribution to the pairing interaction I for the scattered states n and $\bar n$ (= time reversed state to n) of a Cooper pair. A dot (·) indicates a matrix element M and ↑, ↓ indicates the spin contamination.

$$\left.\begin{matrix} I^{\mathrm{dir}} \\ I^{\mathrm{ex}} \end{matrix}\right\} = \sum_{\vec{k},\vec{k}'} \frac{2\hbar\omega_{\vec{k}-\vec{k}'}}{(E_n - E_{n'})^2 - (\hbar\omega_{\vec{k}-\vec{k}'})^2} \times \begin{cases} M(n,n')M(\bar{n},\bar{n}') \\ M(n,\bar{n}')M(\bar{n},n') . \end{cases} \tag{4}$$

We have adopted the usual notation; $M(n,n') = \langle \psi_n \mid \delta V_{\vec{k}-\vec{k}'} \mid \psi_{n'} \rangle$ where $\delta V_{\vec{k}-\vec{k}'}$ is the perturbing potential due to a phonon with momentum $\vec{k}-\vec{k}'$. The matrix elements for direct and exchange scattering are obtained from the wave functions (1) and (2):

$$\begin{aligned} M(n,n') &= M_0(n,n') \left[\cos\frac{\theta}{2}\cos\frac{\theta'}{2} + e^{i(\phi'-\phi)/2}\sin\frac{\theta}{2}\sin\frac{\theta'}{2} \right] , \\ M(n,\bar{n}') &= M_0(n,\bar{n}') \left[e^{-i\phi/2}\sin\frac{\theta}{2}\cos\frac{\theta'}{2} - e^{-i\phi'/2}\cos\frac{\theta}{2}\sin\frac{\theta'}{2} \right] , \end{aligned} \tag{5}$$

where $M_0(n,n') = \langle \phi_n \mid \delta V \mid \phi_{n'} \rangle$. The time-reversed counterparts of (5) are obtained in a similar fashion:

$$M(\bar{n},\bar{n}') = M(n,n')^*, \quad M(\bar{n},n') = -M(n,\bar{n}')^* . \tag{6}$$

I^{dir} and I^{ex} involve products of two M's. The cross terms that arise vanish after averaging over ϕ and ϕ':

$$\langle M(n,n')M(\bar{n},\bar{n}') \rangle_{\phi,\phi'} = |M_0(n,n')|^2 \left[\cos^2\frac{\theta}{2}\cos^2\frac{\theta'}{2} + \sin^2\frac{\theta}{2}\sin^2\frac{\theta'}{2} \right] , \tag{7}$$

$$\langle M(n,\bar{n}')M(\bar{n},n') \rangle_{\phi,\phi'} = -|M_0(n,n')|^2 \left[\cos^2\frac{\theta}{2}\sin^2\frac{\theta'}{2} + \sin^2\frac{\theta}{2}\cos^2\frac{\theta'}{2} \right] . \tag{8}$$

Note that Eq. (8), which is needed for I^{ex}, has a minus sign which will cancel the minus sign in Eq. (3). For this reason direct and exchange terms contribute additively to the binding energy of a *singlet* Cooper pair. On subtracting (8) from (7) one finds identically,

$$\langle M(n,n')M(\bar{n},\bar{n}') \rangle_{\phi,\phi'} - \langle M(n,\bar{n}')M(\bar{n},n') \rangle_{\phi\phi'} = |M_0(n,n')|^2 , \tag{9}$$

so that $I_{nn'}$, Eq. (3), is unaffected by the spin rotations resulting from so scattering. Demonstration of this is the major purpose of this paper.

It is still of interest to determine the changes in I^{dir} and I^{ex}. We estimate these by solving a diffusion equation in spin space. We make the intuitive assumption that the average spin tilt θ can be calculated by keeping track of the stochastic, infinitesimal changes in θ caused by the so term of each scattering event during a coherence time t_ξ.

Let $M(\theta,t)d\Omega$ be the probability of finding a unit vector oriented in the solid angle $d\Omega$ at time t. (We shall treat only the case for which M is independent of ϕ.) The time dependence of M is then given by a diffusion equation on the surface of a sphere as follows:

$$\frac{\partial M(\theta,t)}{\partial t} = D_{\mathrm{so}} \frac{1}{\sin\theta} \frac{\partial}{\partial\theta} \left[\sin\theta \frac{\partial M}{\partial\theta} \right] . \tag{10}$$

D_{so} is a spin-diffusion coefficient, which will be derived below. The solution of (10) is

$$M(\theta,t) = \sum_{l=0}^{\infty} c_l \exp[-l(l+1)D_{\mathrm{so}}t] P_l(\cos\theta) . \tag{11}$$

$\{P_l\}$ are Legendre polynomials. Their coefficients c_l are determined from the initial conditions, which we take to be a δ function along the polar axis, $\theta = 0$. It suffices for our purpose to follow the time evolution of $\langle \cos\theta \rangle$, which determines the so changes of Eqs. (7) and (8). Accordingly, from the $P_1(\cos\theta)$ term of Eq. (11) and the fact that $\langle \cos\theta \rangle = 1$ at $t = 0$, we have after a coherence time t_ξ,

$$\langle \cos\theta \rangle = \exp(-2D_{\mathrm{so}}t_\xi) . \tag{12}$$

The average matrix elements, (7) and (8), are then

$$\langle M(n,n')M(\bar{n},\bar{n}') \rangle_{\phi,\phi'} \approx \tfrac{1}{2} |M_0|^2 [1 + \exp(-4D_{\mathrm{so}}t_\xi)] , \tag{13}$$

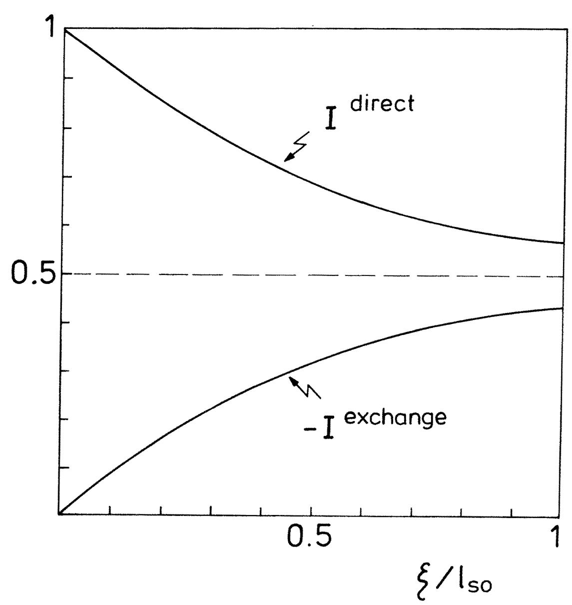

FIG. 2. Direct and exchange parts of the pairing interaction, $I = I^{\mathrm{dir}} - I^{\mathrm{ex}}$, vs ξ/l_{so}; ξ is the effective coherence length and l_{so} is the spin-flip mean free path.

$$-\langle M(n,\bar{n}')M(\bar{n},n')\rangle_{\phi,\phi'}\approx\tfrac{1}{2}|M_0|^2[1-\exp(-4D_{so}t_\xi)]\ . \tag{14}$$

In what follows we shall show that the argument of the exponential factors of (13) and (14) can be expressed in terms of the spin-flip mean free path $l_{so}=\tau_{so}v_F$. (τ_{so} is the spin lifetime.) We will find that

$$2D_{so}t_\xi=\xi/l_{so}\ . \tag{15}$$

The variation of the direct and exchange terms, Eq. (4), with ξ/l_{so} is shown in Fig. 2. Note that the loss in strength of the direct matrix element is compensated by the emergence of the exchange term. In the limit of large so scattering I^{dir} and I^{ex} become equal.[4]

In order to derive Eq. (15) we define the fractional spin polarization, P,

$$P=(N^\uparrow-N^\downarrow)/N\ , \tag{16}$$

where N is the sum $(N^\uparrow+N^\downarrow)$ of spin-up and spin-down electrons. The time variation of P is, of course,

$$\frac{dP}{dt}=\frac{1}{N}\left[\frac{dN^\uparrow}{dt}-\frac{dN^\downarrow}{dt}\right]. \tag{17}$$

Now, let W be the spin-flip probability per scattering event (from an impurity). Since the number of scattering events per second is v_F/l, Eq. (17) implies

$$\frac{dP}{dt}=-2\left[\frac{v_F}{l}\right]WP\equiv-\frac{P}{\tau_{so}}\ . \tag{18}$$

The spin lifetime τ_{so} is, by the above definition,

$$\tau_{so}=\frac{l}{2v_FW}\ . \tag{19}$$

In order to relate τ_{so} to the spin diffusion coefficient D_{so} of Eq. (10), consider the average magnitude, δ, of spin rotation per collision. We take it for granted that $\delta\ll 1$. δ is of course related to W,

$$\cos\delta\cong 1-\tfrac{1}{2}\delta^2=1-2W\ , \tag{20}$$

so $W=\langle\delta^2\rangle/4$. The last equality of Eq. (20) can be seen as follows. Consider a spin rotation δ from an initial spin-up state. After the first collision the probability of spin down is W, and the probability of spin up is $1-W$. Accordingly, $\langle\sigma_z\rangle=(1-W)-W$. The mean-square angular deviation $\langle\Delta^2\rangle$ after n scattering events during a time t is

$$\langle\Delta^2\rangle=n\langle\delta^2\rangle=4D_{so}t\ . \tag{21}$$

The factor 4 is characteristic of two-dimensional diffusion. We eliminate t from (21) by using

$$\frac{n}{t}=\frac{v_F}{l}\ . \tag{22}$$

Whereupon,

$$D_{so}=\frac{v_F}{4l}\langle\delta^2\rangle=\frac{v_F}{l}W\ . \tag{23}$$

We next use Eq. (19) to eliminate W. Thus,

$$2D_{so}=\frac{1}{\tau_{so}}\ . \tag{24}$$

Equation (15) is obtained by multiplying the numerator and denominator of (24) by v_F. The denominator becomes l_{so}, and the numerator is ξ/t_ξ.

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[1] P. W. Anderson, J. Phys. Chem. Solids 11, 26 (1959).

[2] D. Markowitz and L. P. Kadanoff, Phys. Rev. 131, 563 (1963). The band effect is due to a change of $N(0)$, the density of states at the Fermi surface, and other host parameters. The anisotropy effect gives $(\delta T_c/T_c)_{sat}=-\langle a^2\rangle/\lambda$, where λ=BCS parameter and $\langle a^2\rangle$ measures the relative gap anisotropy.

[3] P. W. Anderson, Phys. Rev. Lett. 3, 325 (1959).

[4] R. Hake, Appl. Phys. Lett. 10, 189 (1967). Hake suggests that so scattering can become so strong that $l/l_{so}=\frac{1}{2}$. If $\xi/l_{so}\gg 1$, the direct and exchange contribution to I become of comparable magnitude. Then the spins are completely randomized within ξ. Differentiation between direct and exchange terms then has no physical significance.