SPIN-ORBIT INTERACTION WITH THE LATTICE AND THE KNIGHT SHIFT IN SUPERCONDUCTORS

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It is shown that the spin-orbit interaction with the lattice cannot lead to a large value of the Knight shift in a superconductor. In this connection attention is drawn to the fact that if the shift is independent of the sample size and is equal to $^2/_3$, as in the case of mercury, then this can serve as proof of the fact that Cooper pairing occurs in the triplet state.

IN this short note we discuss the problem of the effect of the spin-orbit interaction of the electrons of the lattice on the Knight shift of a superconductor. We emphasize that we refer specifically to the interaction with the lattice itself, and not to the spin-orbit interaction of the conduction electrons with external impurities or with the boundary of the sample. The latter problem is discussed by a number of authors [1-3] and it has been shown that the Knight shift in a superconductor at absolute zero can have the same value as in the case of a normal metal if the mean free path with respect to spin-flip l_{so} is comparable to the correlation parameter $\xi_0 \sim \hbar v/T_c$. However, the available experimental data (for references cf. [3]) do not demonstrate a dependence of the shift on the sample site d, which enters the mean free path $l_{so} \sim d$. Although the reliability of this assertion can be doubted,[3] it is of interest to investigate the possibilities of the mechanism indicated above which does not involve a dependence on the size in any obvious manner.

As is well known, the Knight shift of the frequency is proportional to the paramagnetic susceptibility:

$$\frac{\Delta\omega}{\omega} = \frac{8\pi}{3N_{at}} |\psi(0)|^2 \chi,$$

where N_{at} is the number of impurity atoms. At $T = 0$ the susceptibility χ of a superconductor vanishes if the spin-orbit interaction is neglected, since the states of the system are classified in terms of their spin and the excited states are separated by a gap. If the spin-orbit interaction is taken into account the spin ceases to be a quantum number, and χ differs from zero.

In order to introduce the spin-orbit interaction with the lattice into the usual scheme of the theory of superconductivity it is necessary to take into account the anisotropy of the metal. Below we shall assume that in addition to the conduction band there exists also an empty band. The spin-orbit interaction has transition matrix elements only between bands involving conservation of quasimomentum, which we shall denote by $\mathbf{L}_p \cdot \sigma$, where σ are the Pauli matrices for the electron spin.

For a normal metal the spin magnetic moment of the conduction electrons in a magnetic field can be calculated in accordance with the usual rules of diagram technique in accordance with Fig. 1:

$$\mathbf{M} \sim \lim_{\mathbf{k}\to 0} T \sum_{\omega} \iint_{\cdot\cdot} \frac{d\sigma_F}{v_F} d\xi \, \mathrm{Sp} \left\{ \sigma_z \mathfrak{G}_{11\omega}\left(\mathbf{p} + \frac{\mathbf{k}}{2}\right) \sigma_z \times \mathfrak{G}_{11\omega}\left(\mathbf{p} - \frac{\mathbf{k}}{2}\right) \right\} \mathbf{H}. \quad (1)$$

(Here M should be considered as the limit in a weak inhomogeneous field ($\mathbf{k} \to 0$) in order to give meaning to the divergent integral in expression (1).) $\mathfrak{G}_{11\omega}(\mathbf{p})$ are the components of the Green's function for the electrons corresponding to an expansion in terms of the Bloch functions and the quasimomentum in the conduction band. In the absence of a spin-orbit interaction the matrix $\hat{\mathfrak{G}}$ is diagonal with respect to the spin indices, and also with respect to the indices of the band number. Naturally, the paramagnetic susceptibility is determined only by the neighborhood of the Fermi surface, i.e., by the first band.

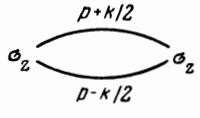


FIG. 1

In the superconducting state the trace in (1) should be replaced by [3]

$$\mathrm{Sp}\{\sigma_z \mathfrak{G}_{11}\sigma_z \mathfrak{G}_{11}\} - \mathrm{Sp}\{\sigma_z{}^t \hat{\mathfrak{F}}_{11}{}^+ \sigma_z \hat{\mathfrak{F}}_{11}\}; \quad (2)$$

$$\mathfrak{G}_{11} = \frac{i\omega + \xi_{1\mathbf{p}}}{\omega^2 + \xi_{1\mathbf{p}}{}^2 + \Delta_{\mathbf{p}}{}^2}, \qquad \hat{\mathfrak{F}}_{11}{}^+ = \frac{\hat{\Delta}_{\mathbf{p}}{}^+}{\omega^2 + \xi_{1\mathbf{p}}{}^2 + \Delta_{\mathbf{p}}{}^2} \quad (3)$$

($\hat{\Delta}_{\mathbf{p}}^+$ is proportional to the metric spinor tensor $\hat{g}_{\alpha\beta} = -\hat{g}_{\beta\alpha}$). As before, $\hat{\mathfrak{G}}$ and $\hat{\mathfrak{F}}^+$ are diagonal in terms of the band indices, with $\mathfrak{F}_{22} = 0$, while $\mathfrak{G}_{22\omega}(\mathbf{p})$ for $\mathbf{p}$ in the neighborhood of the Fermi surface is small:

$$\mathfrak{G}_{22\omega}(\mathbf{p}) \approx -1/D_{\mathbf{p}},$$

where $D_{\mathbf{p}}$ is the separation in energy between the Fermi surface and the empty band ($D \sim 1$ eV).

Substituting (2) into (1) and integrating over ξ we shall obtain for the susceptibility a value proportional to the following integral:

$$\chi \sim \int \frac{d\sigma_F}{v_F} \left\{1 - \Delta_{\mathbf{p}}{}^2 \pi T \sum_{\omega} \frac{1}{(\omega^2 + \Delta_{\mathbf{p}}{}^2)^{3/2}}\right\};$$

at $T = 0$ it vanishes.

We now introduce the spin-orbit interaction which mixes the functions of the various bands. A typical correction in the neighborhood of the Fermi surface for M is shown in Fig. 2a where the double line denotes the Green's function $\mathfrak{G}_{22}$ in the second band. The corresponding contribution to the matrix element is $L_{\mathbf{p}}^2/D_{\mathbf{p}}$. Since the range of integration over ξ and of summation over ω is of order of magnitude Δ, the relative contribution of such corrections is $L_{\mathbf{p}}^2/D_{\mathbf{p}}\Delta_{\mathbf{p}}$ and could become greater if

$$L_{\mathbf{p}}{}^2/D_{\mathbf{p}}\Delta_{\mathbf{p}} \sim 1. \quad (4)$$

Therefore, these corrections should be summed first of all. As regards the nondiagonal components $\mathfrak{G}_{12}$ and $\mathfrak{F}_{12}^+$ arising from the spin-orbit mixing of the bands, their contribution to M is shown in Fig. 2b and, obviously, leads to the following replacement in (1)

$$\sigma_z \to D_{\mathbf{p}}{}^{-2}(\mathbf{L}_{\mathbf{p}}\sigma)\,\sigma_z\,(\mathbf{L}_{\mathbf{p}}\sigma),$$

i.e., to corrections to the g-factor of the electron of order L^2/D^2.

The equations for the functions $\mathfrak{G}_{11}(\mathbf{p})$ and $\mathfrak{F}_{11}^+(\mathbf{p})$ taking spin-orbit corrections (4) into account are shown in Fig. 3. The thick lines correspond to the new functions $\mathfrak{G}$ and $\mathfrak{F}^+$, while the thin lines correspond to expressions (3). However, their solution leads to expressions for $\mathfrak{G}_{11}$ and $\mathfrak{F}_{11}^+$ which differ from (3) by the replacement

$$\xi_{1\mathbf{p}} \to \xi_{1\mathbf{p}} - L_{\mathbf{p}}{}^2/D_{\mathbf{p}},$$

i.e., the effect reduces to a shift of the Fermi surface.

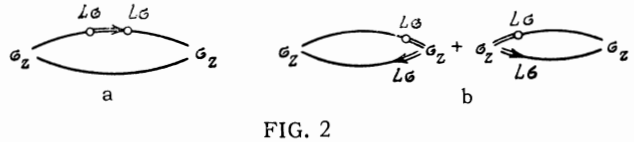
FIG. 3

This negative result is of course explained by the fact that the spin-orbit interaction does not remove the Kramers twofold degeneracy. Therefore, the Fröhlich attraction (due to phonon exchange which gives rise to the Cooper effect and is diagonal in the spins), selects, as before, states of pairs with zero total spin. However, the new Cooper pairs have in their wave function an admixture of the other spin of order L/D. In order to see this we shall now consider the small corrections $\sim$ L/D which arise due to a change in the parameter Δ. Typical expressions are shown in Fig. 4 where the phonon interaction is indicated by a dotted line. Similar terms give a residual Knight shift for a superconductor of the order of

$$L^2/D^2 \ll 1.$$

Thus, the spin-orbit interaction with the lattice is not capable of explaining the observed large value of the Knight shift in superconductors. This result will not be altered if instead of the model considered above we take a superconductor with two overlapping bands. This is associated with the fact that the matrix element of the spin-orbit interaction is diagonal in the quasimomentum as a result of which the shift in the Fermi surface for each of the bands occurs independently. Only the spin-orbit scattering by impurities or by boundaries which has, as has been shown earlier,[3] nondiagonal transitions with respect to the momentum leads to a finite effect.

As already mentioned, experiment shows no dependence on the size of the sample. Moreover, the relative value of the shift χ_S/χ_n in the case of mercury [4] is close to $^2/_3$. The latter value can be easily explained (cf., for example, [5]), if one assumes that the Cooper pairing occurs in the



a b

FIG. 2

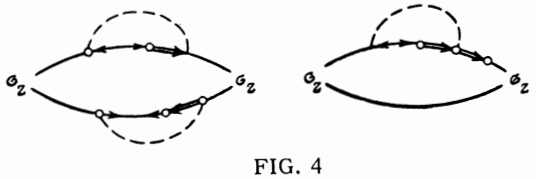


FIG. 4

triplet, and not in the singlet state, as is usually assumed. Therefore, it appears to us that a detailed experimental investigation of this problem would be of great interest.

[1] R. A. Ferrell, Phys. Rev. Letters 3, 262 (1959).

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

[3] A. A. Abrikosov and L. P. Gor'kov JETP 42, 1088 (1962), Soviet Phys. JETP 15, 752 (1962).

[4] F. Reif, Phys. Rev. 106, 208 (1957).

[5] I. A. Privorotskiĭ, JETP 45, 1960 (1963), Soviet Phys. JETP 18, 1346 (1963).

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