Absence of paramagnetic limits for H_{c211} in layered superconductors without inversion center

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It is shown that the reason why the paramagnetic limit of the upper critical magnetic field parallel to the layers is exceeded in the layered superconductors $TaS_2(Py)_{1/2}$ and $NbSe_2$ may be the spin-orbit interaction in a lattice without symmetry center.

According to the experimental data, in the layered superconductors $2H-TaS_2(Py)_{1/2}$ and $2H-NbSe_2$ the upper critical magnetic field H_{c211}, parallel to the layers, exceeds the paramagnetic limit $H_p=\Delta_0/\mu_B\sqrt{2}$ (Δ_0 is the superconducting gap at $T=0$ and μ_B is the Bohr magneton). Thus, in the intercalated compound TaS_2

with pyridine (Py), the superconductivity is not destroyed at $T=1.4\,^\circ$K, in a field $H_{\parallel}=150$ kOe ($T_c=3.25\,^\circ$K and $H_p=60$ kOe).[1] In $NbSe_2$, the paramagnetic effect exerts no influence whatever on the value of $H_{c2\parallel}$, and at $T=1.4\,^\circ$K the field $H_{c2\parallel}$ (~130 kOe) is determined only by the orbital effect ($T_c=7\,^\circ$K and $H_p=130$ kOe).[2]

In principle, the suppression of the paramagnetic effect in layered superconductors may be due to the realization in them of an inhomogeneous state,[3,4] to triplet pairing of the electrons from neighboring layers,[5] and to spin-orbit scattering by impurities. However, the inhomogeneous state and the pairing of the electrons of neighboring layers are sensitive to the scattering of the electrons by impurities within the layers, and these effects are destroyed if the electron mean free path inside the layer is $l \lesssim \xi_0=\hbar v_F/\pi\Delta_0$.[4] According to estimates,[3] in $TaS_2(Py)_{1/2}$ the ratio ξ_0/l ranges approximately from 1 to 6, and the range of variation of ξ_0/l for various $NbSe_2$ crystals is approximately the same. At the same time, experiment revealed no dependence of $H_{c2\parallel}$ on the degree of purity of the samples. Spin-orbit scattering also leads to an appreciable suppression of the paramagnetic effect at an electron mean free path $l_{so} \lesssim \xi_0$ with changing spin, and since $l_{so}/l \lesssim 10^{-2}$, it follows that in layered superconductors $l_{so} \gg \xi_0$ and the spin-orbit scattering changes the paramagnetic limits insignificantly. Moreover, a strong sensitivity of $H_{c2\parallel}$ to the degree of purity of the crystals would be observed in this case.

We shall show below that suppression of the paramagnetic effect in layered compounds can be attributed to spin-orbit interaction of the conduction electrons in a crystal without a symmetry center (in a crystal with a symmetry center, the spin-orbit interaction does not change the properties of the superconductor in a magnetic field[6]). There are certain grounds for assuming that the lattice of a layered superconductor has no symmetry center. The high-temperature $2H$ modifications of TaS_2 and $NbSe_2$ have an inversion center. But when the temperature is lowered, structural metal-metal transitions are observed in these substances, seemingly due to the appearance of a charge-density wave inside the layers.[7] One cannot exclude the possibility that the symmetry center is lost in these transitions (for example, if the charge-density wave is not commensurate with the period of the lattice of the high-temperature phase, the new lattice cannot have a symmetry center). Intercalation of TaS_2 with pyridine suppresses the structure transition, but the pyridine molecules lower greatly the symmetry of the lattice in the plane of the layer, because the dimensions of the molecule are not commensurate with the period of the TaS_2 lattice in the layer.[8]

In a lattice without inversion center, the spin-orbit interaction of an electron with quasimomentum $\mathbf{k}$ can be written in the form $\boldsymbol{\sigma}[\boldsymbol{\epsilon}\times\mathbf{k}]/k_F$. It is shown in[3] that in $TaS_2(Py)_{1/2}$, in a region not close to T_c, the electron motion can be regarded as two-dimensional, and the field $H_{c2\parallel}$ is determined only by the paramagnetic effect. Then the dependence of T_c on $H_{\parallel}$ is determined from the equations

$$g\,\mathrm{Sp}\sum_{\omega}\int d^2\mathbf{k}\,G(\omega,\mathbf{k},\vec{\sigma})\,G(-\omega,-\mathbf{k},-\vec{\sigma})=1,\quad \omega=\pi T(2n+1),$$
$$G^{-1}(\omega,\mathbf{k},\vec{\sigma})=i\omega-\epsilon_0(k)+\vec{\sigma}(\mu_B H+[\vec{\epsilon}_1\times\mathbf{k}]/k_F), \tag{1}$$

where g is the electron-phonon interaction constant and $\epsilon_0(\mathbf{k})$ is the spin-independent part of the electron energy. In layered superconductors, the vector ϵ_1 should lie in the plane of the layers, and then Eq. (1) is transformed at $\epsilon_1 \ll \hbar\omega_D$ into

$$\ln\frac{T_{co}}{T}=2\pi T\sum_{\omega>0}\frac{h^2}{\omega\sqrt{(\omega^2+h^2)(\omega^2+h^2+\epsilon_1^2)}},\quad h=\mu_B H. \tag{2}$$

At $h\gg T_c$ we obtain from (2) an expression for $T_c(H)$

$$T_c(H)=T_{co}(\Delta_0/2Hf)^{\alpha},\quad \alpha=(\sqrt{1+\epsilon_1^2/h^2}-1)^{-1},$$
$$f=2\sqrt{(1+h^2/\epsilon_1^2)(1+2h^2/\epsilon_1^2-2h/\epsilon_1\sqrt{1+h^2/\epsilon_1^2})}. \tag{3}$$

It is seen from (3) that $T_c(H)\neq 0$ at any value of ϵ_1, i.e., there is no paramagnetic limit at $T=0$. At $\epsilon_1\gg T_c$ we have $T_c(H)\approx T_{c0}$ at $h\ll\epsilon_1$, and $T_c(H)$ decreases with increasing H only if $h\gtrsim\epsilon_1$. These results are not sensitive to the scattering of the electrons by the impurities inside the layers. However, the influence of the spin-orbit interaction on the paramagnetic effect depends strongly on the mutual orientation of $\mathbf{H}$, $\boldsymbol{\epsilon}_1$, and $\mathbf{p}$. Thus, if $\boldsymbol{\epsilon}_1$ is perpendicular to the plane of the layers, then at $\epsilon_1\gg T_{c0}$ we obtain $H_{c2\parallel}=\sqrt{2}H_p$ at $T=0$. In the three-dimensional isotropic case, the paramagnetic limit depends on the angle between H and ϵ_1, and the increase of the paramagnetic limit is unbounded as the direction of $\mathbf{H}$ approaches that of $\boldsymbol{\epsilon}_1$.

The proposed model explains the high values of $H_{c2\parallel}$ in $TaS_2(Py)_{1/2}$ and the independence of $H_{c2\parallel}$ of the paramagnetic effect in the low-temperature phase of the anisotropic superconductor $2H-NbSe_2$. We note that the high-temperature phase of $2H-NbSe_2$ can be preserved at low temperatures in a metastable state, this phase is superconducting,[9] and within the framework of our model the paramagnetic effect in this phase should influence $H_{c2\parallel}$ at low temperatures. The spin-orbit interaction in a lattice without symmetry center leads also to the appearance of a Knight shift in the superconducting state,[10] since a direct correlation exists between the excess over the paramagnetic limit and the value of the paramagnetic susceptibility. A strongly anisotropic Knight shift should therefore be observed in $NbSe_2$ and $TaS_2(Py)_{1/2}$ (in the field $H_{\parallel}$, this shift should not change significantly on going from the normal to the superconducting state). All the other mentioned mechanisms for the suppression of the paramagnetic effects yield an isotropic night shift in the superconducting phase.

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