ternal vibrations of polyatomic structural units will be designated as lattice vibrations.

[2)]We use here α and β as the traditional symbols for polymorphic modifications.

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Orientational autolocalization of electrons in multivalley or anisotropic ferromagnetic semiconductors

B. V. Egorov and M. A. Krivoglaz

Institute of Metal Physics, Ukrainian Academy of Sciences

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We consider ferromagnetic semiconductors having a multivalley or essentially anisotropic electron spectrum, in which the energy of the bottom of the band depends, owing to the spin-orbit interaction (SOI), on the direction of the magnetization. It is shown that autolocalized states (AS) of the conduction electrons, due to local changes of the magnetization orientation, can be produced in such crystals. Favorable conditions for the production of these AS obtain in crystals with low magnetic anisotropy, low Curie points, strong SOI, and small distance between the bands. The produced quasiparticles have a large radius and a large effective mass. Their formation leads to a substantial change of the electric and magnetic properties of the crystal and can be regulated by a relatively weak external field and by the temperature.

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A sufficiently strong exchange s–f (or s–d) interaction of the conduction electrons in a ferromagnetic semiconductor with the electrons of magnetic atoms should lead to autolocalization of the conduction electrons at finite temperatures. An electron that happens to be near a fluctuation change of the magnetization is then localized and stabilizes this change by its field.[1-7] The produced autolocalized states (AS) of large radius (fluctuons) are thermodynamically favored if the lowering of the average potential energy of the electron by the localization exceeds the increase of its kinetic energy and of the thermodynamic potential of the spin of the atoms. At $T=0$ the potential energy is minimal even for a band electron at the bottom of the conduction band, and no autolocalization takes place, so that fluctuons are produced in ferromagnets only at not too low temperatures: $T > T_1^*$. In this respect fluctuons differ from polarons in ionic crystals[8] and other AS in ordered systems (with which they have conceptually much in common).

In ferromagnetic semiconductors with anisotropic dispersion law (e.g., in multivalley or uniaxial semiconductors) and with strong spin-orbit interaction (SOI), there can be produced AS of another type, which are stable at low temperatures. When account is taken of the SOI in such semiconductors, the energy of the bottom of the conduction band $E_0(\mathbf{n})$ depends on the orientation of the magnetization vector $\mathbf{M}=M\mathbf{n}$ relative to the crystallographic axes. The equilibrium direction $\mathbf{n}_0$ of $\mathbf{M}$ in the absence of electrons is determined by the magnetic anisotropy of the crystal and does not necessarily correspond to the minimum of $E_0(\mathbf{n})$. Then the average potential energy of the electron can be low-

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ered by rotating, in some region of the crystal, the direction n of the magnetization and by localizing the electron in that region. Obviously, such a rotation of the spins increases the energy of the magnetic anisotropy and the energy of the direct exchange [on account of the produced inhomogeneous distribution of $\mathbf{M}(\mathbf{r})$], and leads also to the appearance of a positive kinetic energy of the electron. However, in weakly anisotropic crystals with low Curie temperatures T_C and with sufficiently large SOI constants the lowering of the electron energy can be larger than the increase of the indicated contribution of the atom spins to the energy, and then the AS near the region of the altered direction of the magnetization (electronic ferromagnetic domain) turns out to be energywise favored and stable. In contrast to fluctuons, the localization here is connected with the local change of the orientation of the vector M, rather than its length, and the region favorable for such an autolocalization can be that of low temperatures $T \to 0$. The corresponding AS can be called orientons. Obviously, in crystals with isotropic dispersion law the dependence of E_0 on n vanishes and the indicated AS should not be produced.

We investigate below the conditions for the formation of such AS and examine their characteristics (the size of the localization region, the energies of the autolocalized states, etc.). To this end we determine first in Sec. 1 the energy $E_0(\mathbf{n})$ of the bottom of the band as a function of the magnetization direction. Analysis shows that the features of the AS differ substantially in cases when $E_0(\mathbf{n})$ depends linearly or quadratically on $\mathbf{n}-\mathbf{n}_0$. The second case takes place if $\mathbf{n}_0$ is perpendicular to the direction $\mathbf{n}=\mathbf{n}_{min}$ for which $E_0(\mathbf{n})$ is minimal. It can be realized, for example, in uniaxial crystals. The first case takes place if $\mathbf{n}_0$ is not perpendicular (and not parallel) to $\mathbf{n}_{min}$. It is more general and is realized, for example, in cubic crystals. The considered AS are much easier to produce in the first case, even for weak SOI, if the magnetic anisotropy is small at the same time. Then the rotations $\delta\theta(\mathbf{r})$ of the spins of the atoms in the AS region, turn out to be small ($\delta\theta \ll 1$). This case will be considered below in Sec. 3 with cubic crystals as the example. In the second case, the AS are produced only for a sufficiently strong SOI, and in them $\delta\theta \sim 1$. Such AS with large spin rotations will be considered in Sec. 4. In Sec. 5 we discuss qualitatively the influence of the temperature and of the external field on orientons, as well as effects connected with defects and with high carrier density.

1. DEPENDENCE OF THE ENERGY OF THE BOTTOM OF THE CONDUCTION BAND ON THE ORIENTATION OF THE MAGNETIZATION

We consider a conduction electron with a wave vector k close to the point $\mathbf{k}_j$ of the energy minimum in the j-th valley of a multivalley semiconductor. The exchange interaction of this electron with the electrons of the unfilled shells of the magnetic atoms H_{sf} will be described with the aid of the s-f (s-d) model of a ferromagnetic semiconductor.[9] We take into account also the SOI H_{sL} of the spin of the conduction electron with its orbital momentum. Then the Hamiltonian of the system can be written in the form

$$H=H_0(\mathbf{r})+H_{sf}+H_{sL}+H_d,$$
$$H_0(\mathbf{r})=-\frac{\hbar^2}{2m_0}\Delta+V(\mathbf{r}); \quad H_{sf}=2\sum_n A(\mathbf{r}-\mathbf{R}_n)\mathbf{s}_e\mathbf{S}_n, \tag{1}$$
$$H_{sL}=\mathbf{s}_e\mathbf{h}; \mathbf{h}=-i\frac{\hbar^2}{2m_0^2c^2}\left[\nabla V(\mathbf{r})\times\frac{\partial}{\partial\mathbf{r}}\right].$$

Here m_0 is the mass of the free electron, $V(\mathbf{r})$ is that part of the periodic potential of the electron which does not depend on the spins of the atoms, s_e and $\mathbf{S}_n$ are the spin operators of the conduction electron and of the n-th magnetic atom (with radius-vector $\mathbf{R}_n$), the δ-like pseudopotential $A(\mathbf{r}-\mathbf{R}_n)$ characterizes the magnitude of the s-f interaction, and the operator H_d describes the direct interaction of the magnetic atoms. We assume for simplicity that they form a Bravais lattice.

The motion of the electron can be considered in the adiabatic approximation, by taking the operators S_n in (1) to be c-vectors. Then the electron Hamiltonian H_e can be written in the form

$$H_e=\sum_{k\sigma}E_k a_{k\sigma}^+ a_{k\sigma}+\frac{2}{N}\sum_{kk'\sigma\sigma'n}A_{kk'}a_{k\sigma}^+\langle\sigma|\mathbf{s}_e\mathbf{S}_n|\sigma'\rangle$$
$$\times a_{k'\sigma'}\exp\{i(\mathbf{k}-\mathbf{k}')\mathbf{R}_n\}+\sum_{\mathbf{k}pp'\sigma\sigma'}a_{kp\sigma}^+\langle kp\sigma|\mathbf{s}_e\mathbf{h}|kp'\sigma'\rangle a_{kp'\sigma'}. \tag{2}$$

The index k designates here the aggregate of the reduced wave vector k and the number p of the band, σ is the spin quantum number, E_k is the energy of the electron in the kp state in the absence of s-f and S-L interactions, $a_{k\sigma}^+$ and $a_{k\sigma}$ are the electron creation and annihilation operators: N is the number of magnetic atoms, and $N^{-1}A_{kk'}$ is the matrix element of $A(r)$ on the wave functions $|k\rangle$ and $|k'\rangle$. For simplicity we confine ourselves hereafter to the case of wide bands, when the band width $\Delta E \lesssim |A_{kk'}|$ (but at low temperatures the results can be used also for the case $\Delta E \lesssim |A_{kk'}|$ by carrying out in the final formulas a certain renormalization of the constants without changing their order of magnitude). We assume also that the SOI energy is small compared with the $S|A_{kk'}|$ and with the energy differences between the different bands.

We regard the last term H_{sL} in (2), which describes the SOI, as a small perturbation. At $T=0$ the spins of the atoms $\mathbf{S}_n=S\mathbf{n}$ are identical and produce a periodic s-f exchange potential, while at $T\neq 0$ such a potential is produced by the average spins $\mathbf{S}_n=\bar{S}\mathbf{n}$. In the field of this exchange potential, the spin of the electron in one of of the state $\sigma=\pm 1$ is parallel or antiparallel to n, and its energy in the zeroth order in H_{sL} and in first order in H_{sf} is equal to $E_k+\sigma\bar{S}A_{kk}$. The first-order correction to the energy in H_{sL} is known[10] to be zero for a ferromagnetic crystal with an inversion center and with a nondegenerate bottom of the band. We consider henceforth crystals with inversion centers, in which the vectors $\mathbf{k}_j$ lie on threefold or fourfold symmetry axes or on the intersection of two symmetry planes. We assume also for simplicity that $A_{pp}<0$.

In the second approximation in H_{sL} we obtain an energy correction that depends on the orientation n relative to the crystal axes. At $\mathbf{k}=\mathbf{k}_j$, according to (2), it is determined by the expression

$$E'=E^{\zeta}_{\mathbf{k}_j p\sigma}=E_0'+2\sum_{i,i'=x,y,z} Q_{ii'}n_i n_{i'}, \tag{3}$$

$$E_0'=\frac{1}{4}\sum_{p'\neq p}\frac{|\langle p\sigma|\mathbf{h}|p'-\sigma\rangle|^2}{E_p-E_{p'}+\sigma\bar{S}(A_{pp}+A_{p'p'})}, \tag{4}$$

$$Q_{ii'}=\frac{1}{8}\sum_{p'\neq p}\left[\frac{\langle p\sigma|h_i|p'\sigma\rangle\langle p'\sigma|h_j|p\sigma\rangle}{E_p-E_{p'}+\sigma\bar{S}(A_{pp}-A_{p'p'})}-\frac{\langle p\sigma|h_i|p'-\sigma\rangle\langle p'-\sigma|h_j|p\sigma\rangle}{E_p-E_{p'}+\sigma\bar{S}(A_{pp}+A_{p'p'})}\right]. \tag{5}$$

All the quantities $\langle p\sigma|h_i|p'\pm\sigma\rangle$, E_p, $A_{pp'}$ are taken here at $\mathbf{k}=\mathbf{k}_j$.

The dependence on $\mathbf{n}$ is determined by the second term of (3), i.e., by the tensor $Q_{ii'}$. If the centers of the valleys lie on three-, four-, or sixfold symmetry axes, then in the coordinate frame in which z is chosen to be a symmetry axis the tensor $Q_{ii'}$ turns out to be reduced to the principal axes, with $Q_{xx}=Q_{yy}\neq Q_{zz}$. Equation (3) then takes the simple form

$$E'=E_0'+2Q_{zz}-2Q\cos^2\theta, \quad Q=Q_{zz}-Q_{xx}. \tag{6}$$

Here θ is the angle between $\mathbf{k}_j$ and $\mathbf{n}$. The quantity Q is determined by Eq. (5). In particular, if $\bar{S}|A_{pp'}|$ are small compared with the characteristic difference of the electron energies $E_e=|E_p-E_{p'}|$ of the different bands (at $\mathbf{k}=\mathbf{k}_j$), then Q is of second order of smallness in E_{SL} and of first order of smallness in A, where E_{SL} and A are the characteristic SOI and s–f exchange energies, respectively. Expanding (5) (including also the matrix elements) in powers of A, we obtain

$$Q=\frac{1}{4}\sigma\bar{S}\sum_{p'\neq p;p''\neq p}\frac{f_{zz}(p,p',p'')-f_{xx}(p,p',p'')}{(E_p-E_{p'})(E_p-E_{p''})}\sim\frac{\bar{S}AE_{SL}^2}{E_e^2}, \tag{7}$$

$$f_{ij}(p,p',p'')=\langle p|h_i|p'\rangle A_{p'p''}\langle p''|h_j|p\rangle.$$

If $\bar{S}|A_{pp'}|$ are large compared with E_0 (e.g., for $4f$ levels), then, according to (5), $|Q|\approx E_{SL}^2/E_e$, where now E_e is the distance between E_p and the nearest subband p'. If the bottom of the band lies at a spectrum-degeneracy point, then Eqs. (3)–(7) are not directly applicable, but E' should depend as before on $\mathbf{n}$, and the change of E' is of order $\bar{S}AE_{SL}/E_e$ larger than in Eq. (7). We note that Eqs. (3), (6), and (7) are valid not only for multivalley but also for single-valley noncubic crystals (at a certain symmetry of the wave functions). In particular, in uniaxial crystals θ designates in this case the angle between $\mathbf{n}$ and the symmetry axis.

To realize the AS of the type considered below, $|Q|$ must be large enough ($|Q|\gtrsim 0.01$ eV). According to (7), favorable substances for this purpose are those with high SOI energies E_{SL} and low E_e. It is known that the SOI increases rapidly with the atomic number of the element, so that E_{SL} is large enough (~0.1–0.3 eV) in compounds of rare earths (and actinides), whereas in compounds of the iron-group elements they are not small if the compounds contain also heavy nonmagnetic atoms at which the amplitude of the wave function is of the same order as at the magnetic atoms. The energies of the direct interband transitions E_e are usually small enough ($E_e\lesssim 1$ eV) in crystals with several atoms per cell and in compounds in which the f-levels are close to the conduction band or to the valence band. For AS ~0.3 eV and $E_{SL}/E_e\sim 1/3$ the estimate (7) yields $Q\sim 0.03$ eV. In the aforementioned case of degenerate minimum points such values of Q can be realized at larger E_e. We note that Q can be determined experimentally by investigating the dependence of the position of the edge of the interband absorption of light for the corresponding direct transition one the orientation of the magnetization (provided that the smearing of the edge does not exceed Q appreciably).

The dependence of the energy of the bottom of the band on the magnetization can be due not only to the "intrinsic" SOI (1), but also to the SOI of the conduction electron with the electrons of the magnetic atoms. In rare-earth compounds the dependence of E' on $\mathbf{n}$ can be due also to Coulomb interaction between the conduction electrons and the $4f$ electrons. Since the S–L interaction is stronger than the crystal field, the external magnetic field earily orients the orbital functions of the $4f$ electrons. This should lead to a substantial dependence of the s–f exchange integral A on $\mathbf{n}$, and hence also to a dependence of the term $\bar{S}A$ in the electron energy, particularly strong (~$0.1\bar{S}A$ at $n_f=6$ or $n_f=8$), if the number of $4f$ electrons is close to 7 or 14 (but is not equal to 7 or 14). According to Ref. 11 the $E(\mathbf{n})$ dependence can be due also to Coulomb interaction with the quadrupole moments of the $4f$ shells. These interactions can make a substantial contribution to Q, which in some cases can exceed (7). We do not present explicit expressions for the corresponding terms in Q (for the last interaction mechanism they are in effect contained in the formulas of Ref. 11), nor the more complicated relations for $E'(\mathbf{n})$, and regard hereafter the total value of Q as a parameter of the theory. We confine ourselves hereafter to systems in which the corresponding Landau energy is much lower than Q.

2. CHANGE OF THE THERMODYNAMIC POTENTIAL OF THE SYSTEM UPON AUTOLOCALIZATION OF AN ELECTRON

The characteristic radius of the AS, as will be shown below, is considerably larger than the lattice constant, i.e., we can use the macroscopic approximation. The state of the electron is then described in the effective-mass approximation. The electron wave function, generally speaking, is a superposition of wave packets pertaining to different valleys. Usually, however, the matrix element $A_{jj'}$ of $A(r-R_n)$ on wave functions of different valleys should not exceed in absolute value the matrix element $A=A_{jj}$ on the wave functions of one valley. In this case, which will be considered later on, it is easy to show (see Ref. 12) that when account is taken of the direct-exchange energy, the state corresponding to a superposition of wave functions from nonparallel valleys is thermodynamically less favored than a state corresponding to a wave packet of functions from one valley or from two parallel valleys. In the last two cases the thermodynamic potential is the same, and for the sake of argument we assume hereafter that the electronic state is made up from wave functions of one valley with wave vector $\mathbf{k}_j$.

To obtain a maximum lowering of the electron energy, the spins of the atoms must be rotated in the xz plane, which contains the vectors $\mathbf{n}_0$ and $\mathbf{k}_j$, and such a coplanar disposition of the spins in the AS in the consider-

ed cases [with U_n given by (11) and (12)] turns out to be thermodynamically most favored. Accordingly, the mean value of the electron spin, becoming attuned to the spins of the atoms, lies in the same plane, and the spinor wave function of the state produced by superposition of waves from the j-th valley can be written in the form

$$\psi_j(\mathbf{r}) = u_{\mathbf{k}_j p}(\mathbf{r})\, e^{i\mathbf{k}_j\mathbf{r}} \begin{pmatrix} \psi(\mathbf{r})\cos{}^1\!/_2\theta_e(\mathbf{r}) \\ \psi(\mathbf{r})\sin{}^1\!/_2\theta_e(\mathbf{r}) \end{pmatrix}. \tag{8}$$

Here $u_{\mathbf{k}_j p}$ is the periodic part of the wave function of a band electron with $\mathbf{k}=\mathbf{k}_j$ (normalized to the volume of the cell), and $\psi(\mathbf{r})$ and $\theta_e(\mathbf{r})$ determine the smooth parts of the spinor wave function of the localized electron.

In the considered systems, for which the typical inequality $|A|S \gg Q$ is satisfied, the direction of the electron spin aligns itself locally with the direction of the magnetization, and at $A<0$ we have $\theta_e(\mathbf{r})=\theta(\mathbf{r})$, where $\theta(\mathbf{r})$ is the angle between the direction $\mathbf{n}(\mathbf{r})$ of the average spins of the atoms at the point $\mathbf{r}$ and the vector $\mathbf{k}_j \| z$ [at $A>0$ we have $\theta_e(\mathbf{r})=\theta(\mathbf{r})-\pi$]. In addition, we confine ourselves first to the case of low temperatures, when only the direction of the magnetization vector changes, but not its modulus ($|\mathbf{M}(\mathbf{r})|=\text{const}$).

With the indicated simplifications, the change $\Delta\Phi$ of the thermodynamic potential of the system following the autolocalization can be represented in the form

$$\Delta\Phi = \min I, \quad I = I[\theta(\mathbf{r}), \psi(\mathbf{r})] = \sum_i \frac{\hbar^2}{2m_i}\int \left|\frac{\partial\psi}{\partial x_i}\right|^2 d\mathbf{r} + \sum_i \frac{\hbar^2}{8m_i}\int \left|\psi(\mathbf{r})\frac{\partial\theta}{\partial x_i}\right|^2 d\mathbf{r} - 2Q\int [\cos^2\theta(\mathbf{r}) - \cos^2\theta_\infty]\psi^2(\mathbf{r})\, d\mathbf{r} + \frac{1}{2}\sum_i \alpha_{ii}\int \left(\frac{\partial\theta}{\partial x_i}\right)^2 d\mathbf{r} + U_a. \tag{9}$$

The first two terms in the formula determine the kinetic energy of the electron, and the third term the potential energy of the SOI, the electron energy level being measured from the bottom of the band at $\mathbf{n}=\mathbf{n}_0$. The fourth term in I determines in the macroscopic approximation the change of the energy of direct exchange of the atom spins. The quantities α_{ii} are connected with the exchange integrals. For example, in crystals with cubic lattices, in the nearest neighbor approximation,

$$\alpha_{xx}=\alpha_{yy}=\alpha_{zz}=\frac{I_0 S^2 a^2}{v} \approx \frac{3SkT_c a^2}{z(S+1)v}, \tag{10}$$

where a is the length of the edge of the cubic cell, $-I_0\mathbf{S}_1\cdot\mathbf{S}_2$ is the exchange energy, v is the volume of the unit cell, and z is the coordination number. The last term in (9) determines the change of the magnetic-anisotropy energy. Retaining for simplicity the lowest harmonics, we can write for U_a in a uniaxial crystal

$$U_a = -\frac{K_1'}{2}\int [\cos^2\theta(\mathbf{r}) - \cos^2\theta_\infty]\, d\mathbf{r}, \quad M^2 \ll K_1' \tag{11}$$

and in a cubic crystal

$$U_a = -\frac{K_1}{2}\int \sum_{i'} (n_{i'}^4 - n_{i'0}^4)\, d\mathbf{r}, \quad M^2 \ll K_1, \tag{12}$$

where K_1' and K_1 are the corresponding anisotropy constants, and x', y', z' are directed along the cubic axes. It is assumed here that $M^2 \ll K_1$ and $M^2 \ll K_1'$. For simplicity, the magnetostatic contribution to U_a is disregarded. If $M^2 \gtrsim K_1$ and $M^2 \gtrsim K_1'$, it is necessary to replace K_1 or K_1' in the result by a quantity $\sim M^2$. AS are more easily produced in crystals with small M^2, for example those containing several nonmagnetic atoms in the cell.

Expression (9) defines $\Delta\Phi$ as the minimum of the functional $I[\theta(\mathbf{r}), \psi(\mathbf{r})]$. The functions $\theta(\mathbf{r})$ and $\psi(\mathbf{r})$, which minimize this functional, specify the stationary distributions of the atom-spin rotation angle $\theta(\mathbf{r})$ and the distribution of the electron density $|\psi(r)|^2$. If $\Delta\Phi = \min I$ is negative, then the autolocalization is certainly thermodynamically favored.

The functional (9) can be minimized by solving the corresponding Euler equations for $\theta(\mathbf{r})$ and $\psi(\mathbf{r})$, or with the aid of a direct variational method for any concrete value of the parameters (e.g., by numerical methods). To present the result in a lucid compact form and to be able to investigate the conditions for the production of the AS and their characteristics in analytic form, we shall carry out the analysis in several typical particular cases in which the solution has a simple approximate form. These examples will be considered in Secs. 3 and 4 below.

3. AUTOLOCALIZED STATES WITH SMALL ROTATION OF THE ATOM SPINS

We consider a crystal whose easy magnetization axis is not parallel or perpendicular to the $\mathbf{k}_j$ direction. An example of such a crystal is a cubic multivalley magnet in which the valleys are oriented along the $\langle 100\rangle$ directions and n_0 is parallel to one of the $\langle 111\rangle$ axes, or conversely, $\mathbf{k}_j \| [111]$ and $\mathbf{n}_0 \| [100]$. For simplicity we confine ourselves to the case when the difference between the components m_i of the effective-mass tensor is small, and, neglecting terms quadratic in $m_1 - m_3$, we replace m_i by $m=(m_1 m_2 m_3)^{1/2}$ (in noncubic crystals, we shall assume the difference of the quantities $\alpha_{ii}m_i$ to be small and replace also α_{ii} by $\alpha = \sum \alpha_{ii} m_i/m$). We assume that the constants of the SOI Q and of the magnetic anisotropy are small, as a result of which AS are produced with small rotation of the atom spins. This allows us to discard the second term in (9) and reduce $I[\theta, \psi]$ to a quadratic form of $\theta(\mathbf{r}) - \theta_\infty$. Minimization with respect to $\theta(\mathbf{r})$ leads then to the Euler equation

$$\alpha\Delta\theta - 2Q\psi^2 \sin 2\theta_\infty - 2K_1\zeta(\theta - \theta_\infty) = 0, \tag{13}$$

where $\zeta = 1$ at $\mathbf{n}_0 \| [100]$, $\zeta = -\frac{2}{3}$ at $\mathbf{n}_0 \| [111]$, and $\zeta \sim 1$ for noncubic crystals. It is easy to solve this equation and express $\theta(\mathbf{r})$ in terms of $\psi(\mathbf{r})$, for example with the aid of a Fourier transformation.

To determine the minimum of the functional $I[\psi]$, which is obtained after substituting the solution (13) in (9), we use a direct variational method and use for $\psi(\mathbf{r})$ the usual simple approximation

$$\psi(\mathbf{r}) = (2\beta/\pi)^{3/4}\exp(-\beta r^2). \tag{14}$$

Then the functional $I[\psi] = \min_\theta I[\theta, \psi]$ reduces to the function

$$I(\beta) = \frac{3}{2}\frac{\hbar^2\beta}{m} - \frac{2}{\pi^2}\beta^{1/2}\frac{Q^2}{\alpha}\sin^2 2\theta_\infty \int_0^\infty \frac{x^2\exp(-x^2)\,dx}{x^2 + \zeta K_1(2\alpha\beta)^{-1}}. \tag{15}$$

After determining the value $\beta=\beta_0$ corresponding to the minimum of (15) we can obtain the change $\Delta\Phi=I(\beta_0)$ of the thermodynamic potential following autolocalization, the energy E of the localized electron, as well as the number $n=v^{-1}\psi^{-2}(0)$ of the magnetic atoms in the electron localization region and the maximum atom spin rotation $\delta\theta=\theta(0)-\theta_\infty$. The analysis becomes much simpler if the magnetic anisotropy constant K_1 is small enough (as is frequently the case in cubic crystals). If the anisotropy can be neglected, then $I(\beta)$ is described schematically by curve a of Fig. 1, i.e., the AS are produced without overcoming an energy barrier, and $\Delta\Phi=I(\beta_0)$ is always negative, i.e., the AS is energywise favored. Its equilibrium characteristics are determined by the formulas

$$\begin{aligned}\Delta\Phi&=\frac{1}{3}E=-\frac{5g^4}{6\pi^3}\frac{Q^4}{I^2\Delta E}=\frac{gQ\delta\theta}{2^{1/2}},\\ n&=\frac{27\pi^6}{250\cdot 2^{1/2}}\frac{I^3(\Delta E)^3}{g^6Q^6}=\frac{3}{5\cdot 2^{1/2}}\frac{1}{(\delta\theta)^2}\frac{\Delta E}{I},\\ \delta\theta&=-\frac{5\cdot 2^{1/2}}{3\pi^3}\frac{g^3Q^3}{I^2\Delta E}\ll 1 \quad \text{at} \quad K_1vI(\Delta E)^2\ll Q^4,\end{aligned} \tag{16}$$

where

$$\Delta E=\frac{5\hbar^2}{mv^{2/3}},\quad g=\sin 2\theta_\infty,\quad I=\alpha v^{1/3}.$$

We have introduced here in lieu of m the energy constant ΔE (which is close to the width of the conduction band in single-valley crystals), and in lieu of α the energy constant $I\sim(1-3)I_0S^2\sim(0.3-0.6)kT_C$. In cubic crystals $\cos\theta_\infty=3^{-1/2}$ and $g^2=\frac{8}{9}$.

When the magnetic anisotropy is taken into account, the $I(\beta)$ curves (curves b and c of Fig. 1) pass through a maximum of height

$$q=\frac{\pi^3}{250}\frac{(\zeta K_1v)^2}{(gQ)^4}(\Delta E)^3 \quad \text{at} \quad K_1\ll K_1^*;$$

this height characterizes the energy barrier for the transition into the AS. With increasing K_1, $\Delta\Phi$ increases, and at $K_1>K_1^*$ (K_1^* corresponds to curve c on Fig. 1), $\Delta\Phi$ becomes positive, the formation of the AS as $T\to 0$ becomes energywise unprofitable. It follows from (15) that

$$K_1^*=0.1g^4Q^4/I(\Delta E)^2v. \tag{17}$$

According to (17), crystals suitable for the realization of the AS of the considered type are those with small anisotropy, low Curie points, large effective masses, and not too small Q. For example at $\zeta=1$, $Q=0.03$ eV, $I=2.10^{-3}$ eV, $v=3.10^{-23}$ cm^3 ($z=6$; $S=2$, $T_C\approx 70$ K), and $\Delta E=1.4$ eV ($m=3m_0$) the AS are produced if $K_1<K_1^*\approx 9.10^5$ erg/cm^3. At $K_1\ll K_1^*$ and at the cited values of the parameters, according to (16), we have $\Delta\Phi=-3.10^{-3}$ eV, $\delta\theta=-0.3$, $n=3.10^3$. In this case $-E=9\times 10^{-3}$ eV $>kT_C\gg kT$.

At sufficiently large Q and small I and ΔE, the condition $\delta\theta\ll 1$ no longer holds. The characteristics of the AS at large $\delta\theta$ will be considered in the next section. So long as $\delta\theta\ll 1$, the quantity n is large (usually $\Delta E/I>10^3$), and the condition of applicability of the macroscopic approximation is well satisfied.

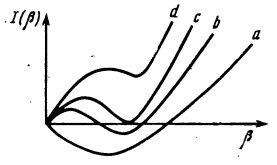

FIG. 1.

To satisfy also in the case $\Delta E\gg AS$ the adiabatic approximation used above, the electron energy $|E|$ must be large both compared with kT (with the energy of the really excited magnons), and compared with the energy of magnons having a wave vector $\sim\beta^{1/2}$ (of the order of the reciprocal dimension of the AS). At $K_1\ll K_1^*$ the last condition reduces to the requirement $\Delta E\gg I$ or $m\ll m_m$ (m_m is the magnon mass), which is almost always satisfied.

The considered AS are quasiparticles having an effective mass M. The latter can be obtained by the method used to calculate the effective mass of the polaron,[13,8] by determining $\Delta\Phi$ for a quasiparticle moving with velocity v and described by the functions $\psi(\mathbf{r}-\mathbf{v}t)$, $\theta(\mathbf{r}-\mathbf{v}t)$. In the case $\delta\theta\ll 1$, $K_1\ll K_1^*$ and $\mathbf{v}\to 0$, calculation at $\mathbf{n}_0\parallel[100]$ leads to the expression

$$\frac{M}{m}=\frac{3\cdot 2^{1/2}}{40\pi}\frac{S^2\Delta E(gQ)^2}{I^{7/2}(vK_1)^{1/2}}\sim\frac{1}{10}\left(\frac{K_1^*}{K_1}\right)^{1/2}\left(\frac{S\Delta E}{I}\right)^2. \tag{18}$$

For example, for the parameters given above and at $K_1=10^5$ erg/cm^2 we have $M/m_0\approx 0.6\times 10^6$.

It must be borne in mind, however, that Eq. (18) was obtained in a continual approximation. Even the weak influence of the lattice periodicity on the transational motion of the quasiparticle leads to the appearance of forbidden bands in the $\Delta\Phi(\mathbf{p})$ spectrum ($\mathbf{p}$ is the total momentum of the system), and at such large M the widths of these bands can exceed those of the allowed bonds, $\sim\Delta Em/M$, corresponding to the mass (18) calculated without allowance for the periodic potential. In this case Eq. (18) can no longer be used. The motion of quasiparticles with such large M at all T except the very lowest is apparently of the diffusion type.

4. AUTOLOCALIZED STATES WITH LARGE ATOM SPIN ROTATION

The AS considered above with $\delta\theta\ll 1$ cannot occur at all in crystals where $\mathbf{n}_0\perp\mathbf{n}_{min}$, i.e., where the energy of the bottom of the band at small $\delta\theta$ depends on $\theta-\theta_\infty$ not linearly but quadratically. In these cases there can be produced only AS with almost complete alignment of the atom spins with the electron spin. We shall investigate such states using as an example uniaxial magnets with two minima of the electron spectrum on the z axis or with one minimum at $\mathbf{k}=0$, for which the easy magnetization axis $\mathbf{n}_0\parallel z$ ($K_1'>0$) and $Q<0$, or else $\mathbf{n}_0$ lies in the xy plane ($K_1'<0$) and $Q>0$. The results, with some change in notation, are applicable also to cubic crystals with large Q. Just as above, we shall assume that $\alpha_{11}m_1\approx\alpha_{33}m_3$ and, neglecting the terms $\sim(\alpha_{11}m_1-\alpha_{33}m_3)^2$, replace in (9) m_i by m and α_{ii} by α.

At large $\delta\theta$ it is much more difficult to determine the $\delta\theta(\mathbf{r})$ corresponding to a given distribution $\psi(\mathbf{r})$ than in the case $\delta\theta\ll 1$. It is therefore more convenient to minimize the functional $I[\theta,\psi]$ by a direct variational

method, specifying the trial function $\theta(\mathbf{r})$ of the angular deviation from the z axis. We specify it by means of the relation

$$\cos^2\theta(\mathbf{r})-\cos^2\theta_\infty=t/\mathrm{ch}^2\gamma r, \quad |t|\leqslant 1. \tag{19}$$

The chosen function contains two varied parameters and accounts correctly for the general course of the function $\theta(\mathbf{r})$, but decreases rapidly as $r\to\infty$. In the parameter region where $\Delta\Phi\approx 0$, this approximation leads to an error ~10–20%, but with increasing $|\Delta\Phi|$ the error decreases rapidly (with the calculated value of $\Delta\Phi$ overestimated).

When (9) and (19) are taken into account, $\psi(\mathbf{r})$ and the electron energy E can be obtained by determining the minimum of the functional

$$E[\psi(\mathbf{r})]=\frac{\hbar^2}{2m}\int|\nabla\psi|^2d\mathbf{r}+\frac{\hbar^2\gamma^2}{8m}\int\frac{|\psi|^2}{\mathrm{ch}^2\gamma r}d\mathbf{r}$$
$$-\frac{\hbar^2\gamma^2}{8m}(1-|t|)\int\frac{|\psi|^2(1+|t|\mathrm{th}^2\gamma r)}{\mathrm{ch}^2\gamma r-|t|}d\mathbf{r}-2Qt\int\frac{|\psi|^2d\mathbf{r}}{\mathrm{ch}^2\gamma r}. \tag{20}$$

It will be shown below that an equilibrium AS correspond to values of $|t|$ very close to unity. This makes it possible to discard the third term in (20). The corresponding error does not exceed 5%. The definition of the minimum of the functional (20) without the third term corresponds to a solution of the Schrödinger equation with a potential proportional to $\cosh^{-2}\gamma r$. Taking into account the known relation between the solutions of the spherically symmetrical problem with $l=0$ and the antisymmetrical solutions of the one-dimensional problem, we can write down the expression for E in the form (see, e.g., Ref. 14)

$$E(t,\lambda)=-2Qt(1-1/2\lambda)^2, \quad \lambda=4mQt/9\hbar^2\gamma^2. \tag{21}$$

Replacing the first three terms in (9) by expression (21) and calculating the last two terms in (9), and taking into account (11) and (19) and the definitions (16) of I and ΔE, we express $\Delta\Phi$ in the form

$$\Delta\Phi=\min I(t,\lambda), \quad I/2|Q|=-t\left(1-\frac{1}{2\lambda}\right)^2+C\frac{\lambda^3}{|t|^{1/2}}$$
$$+C_1\frac{\lambda}{|t|^{1/2}}\left[1-\left(\frac{1-|t|}{|t|}\right)^{1/2}\tau\left(1-\frac{3\tau}{2\pi}+\frac{\tau^2}{2\pi^2}\right)\right],$$
$$\tau=\arccos(2|t|-1), \quad C=\frac{9\pi^3}{160\cdot5^{1/2}}\frac{K_1'v}{|Q|}\left(\frac{\Delta E}{|Q|}\right)^{3/2}, \tag{22}$$
$$C_1=\frac{\pi^3}{8\cdot5^{1/2}}\frac{I}{|Q|}\left(\frac{\Delta E}{|Q|}\right)^{1/2}.$$

The parameter λ is connected with the effective γ^{-1} radius of the AS and with the effective number $\tilde{n}$ of the atoms in the region of the changed $\cos^2\theta$:

$$\tilde{n}=\frac{\pi^3}{3\gamma^3v}=9\left(\frac{\pi^2\lambda^2}{20t}\frac{\Delta E}{Q}\right)^{1/2}, \quad \gamma v^{1/3}=\frac{2\cdot5^{1/2}}{3\lambda}\left(\frac{Qt}{\Delta E}\right)^{1/2}. \tag{23}$$

In the considered case, in contrast to the case dealt with in Sec. 3, the $I(\gamma)$ curves (even if we neglect the magnetic anisotropy) always have maxima and they have the same shape as curves b–d (but not a) of Fig. 1. Therefore $\Delta\Phi=\min I$ becomes negative and the AS are stable as $T\to 0$ only in a definite range of values of the parameters at sufficiently large Q. Numerical calculations show that the stability region lies to the left of the curve shown in Fig. 2. The transition to the AS involves in this case the surmounting of an energy barrier.

For a more detailed investigation of the characteris-

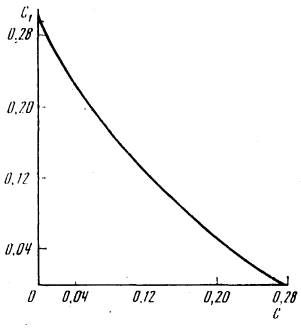

FIG. 2.

tics of the AS let us examine limiting cases in which the change of the magnetic-anisotropy energy by autolocalization is either much larger or much smaller than the change of the energy of the direct exchange. In the first case, when $C\gg C_1$, the last term of (22) can be discarded. Then the smallest value of I is reached at $|t|=1$, i.e., the angle of rotation at the center of the AS is $\theta-\theta_\infty=\pm\pi/2$ [in this case Eq. (21) determines the exact value of $\lambda=\lambda_0(C)$ for a potential energy in the form (19)]. The stationary value of $\lambda=\lambda_0(C)$ is determined by the equation $6C\lambda^5=2\lambda-1$, whose solution makes it possible then to obtain from Eqs. (21)–(23) the values of E, $\Delta\Phi$, γ, and $\tilde{n}$ as functions of C. The AS are energywise favored ($\Delta\Phi\leqslant 0$) at $C\leqslant C^*$, where

$$C^*=0.28, \quad \lambda_0(C^*)=5/6, \quad E(C^*)=-0.32|Q|, \quad \gamma(C^*)=1.8(|Q|/\Delta E)^{1/2}v^{-1/3},$$
$$\tilde{n}=1.8(\Delta E/|Q|)^{3/2} \quad (C^*\gg C_1). \tag{24}$$

According to (24), $\tilde{n}(C^*)$ is very large, i.e., the macroscopic approximation is valid. With decreasing C, the values of $\tilde{n}$, $\Delta\Phi$, and E tend to the asymptotic expressions

$$\Delta\Phi=-2|Q|\left(1-\frac{4}{3}(3C)^{1/4}\right); \quad E=-2|Q|[1-(3C)^{1/4}],$$
$$\tilde{n}=9\left(\frac{\pi^2}{20(3C)^{1/3}}\frac{\Delta E}{|Q|}\right)^{1/2} (C_1\ll C\ll C^*). \tag{25}$$

For example, at $v=3\times10^{-23}$ cm^3, $Q=0.03$ eV, and $\Delta E=4.3$ eV ($m=m_0$) the condition $C\leqslant C^*$ is satisfied and the AS are stable if $K_1'<6.2\times10^5$ erg/cm^3 and $n(C^*)=3\times10^3$. Simultaneously, $C^*\gg C_1$ and we can neglect the contribution of the direct exchange to $\Delta\Phi$ if $I\ll10^{-3}$ eV (i.e., $T_C\ll35$ K at $z=6$).

In the opposite limiting case $C\ll C_1$ we can neglect the change of the magnetic-anisotropy energy and discard the second term of (22). In this case the minimum of $I(t,\lambda)$ is reached at $|t|=t_0$ somewhat smaller than unity (the spin rotation angle at the center of the AS does not reach the maximum value), and $\Delta\Phi\leqslant 0$ at $C_1\leqslant C_1^*$, where at $Q>0$ we have

$$C_1^*=0.30, \quad t_0(C_1^*)=0.93, \quad \lambda_0(C_1^*)=3/2, \quad E(C_1^*)=-0.83Q,$$
$$\gamma(C_1^*)=0.96(Q/\Delta E)^{1/2}v^{-1/3}, \quad \tilde{n}(C_1^*)=12(\Delta E/Q)^{3/2} \quad (C\ll C_1^*). \tag{26}$$

With decreasing C_1, the parameter t_0 tends to unity and λ_0, neglecting $1-t_0$, is a solution of the equation $2C_1\lambda^3=2\lambda-1$. At small $C_1\ll C_1^*$ and $C\ll C_1$ we have

$$\Delta\Phi=-Q(1-2C_1^{1/2}), \quad E=-Q(1-C_1^{1/2}), \quad \tilde{n}=9\left(\frac{\pi^2}{20}\frac{\Delta E}{C_1Q}\right)^{1/2}. \tag{27}$$

For example, at $v=3\times10^{-22}$ cm^3, $Q=0.03$ eV, and

$m = m_0$ the AS are produced ($C_1 < C_1^*$) if $I < 2.2\times10^{-3}$ eV, i.e., at sufficiently low T_C ($T_C < 75$ K at $z=6$ and $S=2$) and at small $K_1' \ll 8\times10^4$ erg/cm^3 (so as to have $C \ll C_1^*$). At $C_1 = C_1^*$ we obtain $n = 2\times10^4$. Just as in Sec. 3, the condition for the applicability of the adiabatic approximation reduces to the requirement $|E| \gg kT$ and $|E| \gg I$.

The presented results, which describe almost a complete spin flip ($t_0 \approx 1$), are valid in fact not only for uniaxial crystals with the considered valley geometry, but also to other cases of large $Q[Q^3 \gg I^2\Delta E, Q^5 \gtrsim \Delta E^3(K_1'v)^2]$, for example to cubic crystals. In the latter case, at a small magnetic anisotropy, $I(t, \lambda)$ can be also estimated (with a 20% error) from formula (22) (without the second term), by replacing in it C_1 by $C_1(1-\cos\theta_\infty)^{-1/2}$. Accordingly the AS are described in this case by Eqs. (26) and (27), in which the indicated substitution is made.

5. DISCUSSION OF RESULTS

It follows from the cited results that the character of the formation of the AS is substantially different in the cases when the magnetization axis $\mathbf{n}_0$ makes an acute or a right angle with the direction $\mathbf{n}_{min}$ corresponding to the minimum energy of the bottom of the band [the electron potential energy $Q(\cos^2\theta = \cos^2\theta_\alpha)$ is a linear or quadratic function of $\delta\theta$ at small $\delta\theta$]. In the second case, which is realized, for example, at the considered geometry of the valleys in a uniaxial crystal, the AS are produced, even at extremely small magnetic anisotropy K_1', only starting with certain finite values of the coupling constant Q, and after surmounting an energy barrier. They are similar in many respects to the AS in liquid helium and to fluctuon states in disordered systems. In the former case, which is realized in cubic crystals, in uniaxial crystals with valleys lying in the easy-magnetization plane x', y', and in a number of low-symmetry crystals, the AS are produced in the limit as $K_1 \to 0$ at arbitrarily small $|Q|$ and there is no energy barrier. The produced AS with $\delta\theta \ll 1$ have many features in common with large-radius polarons in ionic crystals. At the same time, the difference between the dispersion laws of the phonon and magnon frequencies and between the constants of their interaction with electrons leads to substantial differences of the AS (as well as of the impurity optical spectra[15]). In particular, in magnets, unlike in polarons, the condition of applicability of the adiabatic approximation is satisfied even in the case of weak coupling.

The considered AS are apparently most readily realized in cubic crystals with small magnetic anisotropy, with low Curie points, with large effective masses and with appreciable $|Q|$ ($\gtrsim 10^{-2}$ eV). The last condition, according to (17), is particularly important.

Although the described results were obtained for the case $T=0$, they are applicable also at finite temperatures [when the change of the modulus of $\mathbf{M}(\mathbf{r})$ in the region of the AS can still be neglected], if account is taken of the temperature dependence of the parameters. According to (7), $Q \sim \bar{S}$ decreases with increasing T, and this can lead to a transition from the AS to band states in a certain region $T \sim T^*$. At $\mathbf{n}_0 - \mathbf{n}_{min}$ or at appreciable K_1, it has the features of a smeared first-order transition. On the other hand, I, and also in particular K_1, decrease with increasing T. Therefore cases are possible when no AS are produced at $T=0$, and they are thermodynamically favored only in the interval $0 < T_1^* < T < T^*$. Starting with certain temperatures, usually $\sim T_C/3$ to $T_C/2$, an important role can be played also by the change of the modulus of $\mathbf{M}(\mathbf{r})$ in the AS region, and mixed states of the fluctuon type can be produced, in which both the magnitude and direction of $\mathbf{M}$ are changed. A transition can then take place from states with very large radius, where the change of $|\mathbf{M}|$ is small, into states of smaller radius with appreciable change of $\mathbf{M}(\mathbf{r})$.

The transition of the electrons into the considered AS should obviously alter substantially the electric, photoelectric, magnetic, and other properties of the crystals (the carrier mobility, their density, kinetic characteristics, magnetic anisotropy, etc.). It is possible to alter significantly these properties by applying a relatively weak external field H, on the order of the anisotropy field. By rotating the magnetization, the field can easily destroy the AS (at $\mathbf{n}_0 \parallel \mathbf{n}_{min}$) or lead to appearance of AS (when $\mathbf{n}_0$ makes an acute angle with $\mathbf{n}_{min}$). An oblique field makes possible AS with $\delta\theta \gg 1$ in uniaxial crystals. The field can decrease effectively the anisotropy and facilitate the formation of the AS, inasmuch as in the presence of a field the quantity $K_1\zeta$ in the formulas of Sec. 3 is replaced by $\tilde{K}/2$, where $\tilde{K} = \partial^2(U_a - \mathbf{M}\cdot\mathbf{H})/\partial\theta^2$. It is known that $\tilde{K} \to 0$ at certain H, making the conditions for the formation of AS at $T \to 0$ most favorable.

Even if the free electrons do not go over into the AS, regions of reversed magnetization in crystals with anisotropic spectra should appear near electronic impurity center. They should lead, in particular, to an appreciable electronic contribution to the magnetic-anisotropy constant and to the broadening of the ferromagnetic-resonance line. New effects should appear at considerable carrier densities N_e. Upon increase in density there can occur, in particular, electronic phase transitions accompanied by reversal of the magnetization or by formation of a heterogeneous state with a nonuniform distribution of $\mathbf{M}(\mathbf{r})$ and $N_e(\mathbf{r})$.

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Study of two-dimensional mixed state of type-I superconductors

I. L. Landau and A. E. Svistov

Institute of Physics Problems, USSR Academy of Sciences
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We describe an experimental study of the destruction of superconductivity by current in hollow indium samples. In particular, we determine the destruction current I_{c2} of the two-dimensional mixed state and investigate the temperature dependence of the paramagnetic effect in a weak longitudinal magnetic field. In addition, we investigate the mixed state produced on the surface of a bulky cylindrical sample when a strong longitudinal magnetic field is abruptly turned off. Particular attention is paid to the study of the structure produced in a two-dimensional mixed-state layer in the presence of a weak transverse magnetic field. The velocity and the characteristic dimensions of the structure are measured at various values of the temperature and current density in the sample and of the transverse magnetic field.

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Destruction of the superconductivity of hollow type-I superconductors by current produces on their inner surface a thin layer of two-dimensional mixed (TM) state (private communication from L. D. Landau to D. Shoenberg, see Refs. 1 and 2). The TM state has been the subject of a number of experimental[2–9] and theoretical[10–15] studies. Nontheless, many questions connected with the properties of the TM state remain unanswered to this day.

This paper consists of two methodologically different parts. In the first are described experimental study of the TM state produced on the inner surface of a hollow cylindrical sample. In particular, the current I_{c2} required to destroy the TM state has been measured. In addition to measurements of I_{c2}, we have investigated the temperature dependence of the paramagnetic effect of the TM state in a longitudinal magnetic field.

In the second part are described experimental studies of the TM state produced on the surface of a bulky cylindrical sample when an external magnetic field is turned off. This experiment, proposed by Dolgopolov and Dorozhkin,[6] is methodologically somewhat simpler than the destruction of the superconductivity of hollow cylinders by a current. On the other hand, the damping of the vortical currents produces in the TM-state layer nonstationary external conditions, thereby limiting somewhat the experimental possibilities. Particular attention was paid in the described experiments to the study of the structure produced in the TM state layer in a transverse magnetic field.

1. DESTRUCTION OF THE SUPERCONDUCTIVITY OF HOLLOW INDIUM CYLINDERS BY A CURRENT

Experimental setup

We used for the measurements two single-crystal samples[1)] with identical dimensions: outside diameter 8 mm, inside diameter 4 mm, and length 55 mm. The tetragonal axis was parallel to the sample axis. The resistance ratio $R_{300\ K}/R_0$ was 1700 and 1300 for samples 1 and 2 respectively. The currents through the samples (up to 1200 A) were produced by a current transformer with superconducting windings in accord with a previously described procedure.[4] The mounting of the samples is illustrated in Fig. 1. Two pairs of Helmholtz coils 4 and a solenoid 5, located in the immediate vicinity of the sample, could produce at the sample a magnetic field of any strength and direction.

The current needed to destroy the TM state was determined by measuring the surface impedance, using two coils $L1$ and $L2$. The coils were flat spirals and had approximately 40 turns of copper wire of 20 μm diameter each. The approximate dimensions of the coils and their arrangement in the sample cavity are shown in Fig. 1. The coils were connected in the tank circuit of a measuring rf oscillator, whose change of frequency was measured (and was proportional to the changes of the imaginary part of the surface impedance) as the state of the sample was varied. The oscillator frequency in these experiments was ~10 MHz, and the change of frequency $f_s - f_n$ when the sample went from

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