Helical phases in superconductors

V. P. Mineev and K. V. Samokhin

L. D. Landau Institute of Theoretical Physics, Russian Academy of Sciences, 117334 Moscow, Russia

In this paper we analyze the consequences of introducing terms that are first order in the spatial gradient (Lifshits invariants) into the Ginzburg–Landau functional for superconductors. Invariants of this kind can be considered both for superconductors without a center of inversion, where the Lifshits invariant is introduced in the standard way, and for superconductors with a center of inversion, where the Lifshits invariant is constructed out of two different irreducible representations of the crystal symmetry group that differ in their spatial parities. When terms that are linear in the gradient are included in the Ginzburg–Landau functional helical superconducting phases appear. We investigate the thermodynamic and magnetic properties of these phases, and also the extent to which they can address the problem of splitting of the superconducting phase transition in UPt$_3$.

1. INTRODUCTION

Experimental discoveries in recent years in the area of new superconducting materials, such as, e.g., the "heavy-fermion" superconductors (see the review by Gor'kov[1]), have stimulated the theoretical investigation of models with multicomponent order parameters and superconducting phases with complex structures.

A prominent role in this theory is played by the symmetry approach,[2] which is based on the properties of the full symmetry group $G = G_0 \times R \times U(1)$ of the superconductor where G_0 is the point group of macroscopic symmetries of the crystal, R is the operation of time reversal, and $U(1)$ is the group of gauge transformations.

Each superconducting phase has an order parameter that transforms according to one of the irreducible representations of the group G_0, i.e., that can be written in the form of a linear combination of functions that form a basis for the corresponding irreducible representation. The specific form of the coefficients in this linear combination is found by minimizing the Ginzburg–Landau functional for the free energy, which is an invariant with respect to transformations of the group G. The set of symmetry operations that leave invariant the state (order parameter) of a given superconducting phase form a group H (or superconducting class) which is a subgroup of the group G. Any one of the groups H is isomorphic to one of the subgroups H_0 of the group G_0 of macroscopic crystal symmetries, and consists of transformations H_0 combined with various gauge transformations from $U(1)$ (multiplication by a phase factor) and the operation of time reversal.

Thus, the original symmetry of the crystal is lowered as a result of a phase transition to the superconducting state. The transition to an ordinary superconducting state, whose order parameter transforms according to the unit representation of the group G_0, is accompanied only by breaking of gauge invariance, i.e., $G = G_0 \times R \times U(1)$, $H = G_0 \times R$. Phases whose appearance breaks the directional symmetry of the crystal or the symmetry under time

reversal R (magnetic superconductors) are customarily called unusual superconducting phases.

As for the operation of spatial parity, all the currently known "heavy fermion" compounds that seem to exhibit unusual superconductivity possess a center of inversion, i.e., $G_0 = \bar{G}_0 \times C_i$, where $\bar{G}_0$ is the group of macroscopic rotation symmetries and C_i is the operation of spatial inversion. This property is apparently preserved in the superconducting state as well, i.e., the superconducting order parameters possess a definite spatial parity. In other words, Cooper pairing takes place only in a spatially even state (spin singlet) or in a spatially odd state (spin triplet). The classification of unusual superconducting phases given by Volovik and Gor'kov[2] presumes the presence of a center of inversion. This prevents both the appearance of terms of first order in the gradient (Lifshits invariants) in the Ginzburg–Landau functional and the existence of nonuniform (helical) superconducting phases, as well as the appearance of superconducting phases that do not possess a definite parity.

However, recent experimental data suggests that the crystal structure of UPt$_3$ is more complicated than previously assumed. Data on electron Bragg scattering[3] show the presence of several density waves that are incommensurate with the hexagonal lattice. The interaction of these structural modulations with the orthorhombic deformation tensor and the polarization of the crystal lead, after averaging over a volume with dimensions much larger than the superstructure period, to the appearance of nonzero deformations and polarizations. This, in turn, changes the macroscopic directional symmetries of the original crystal (i.e., the crystal class), which has the following consequences, as shown by Mineev:[4] first of all, the symmetry is lowered from hexagonal to orthorhombic, which from the point of view of superconductivity is equivalent to including an external field with symmetry D_{2h} that splits the superconducting transition; and secondly, the crystal loses its invariance with respect to spatial inversion, which can lead to the appearance of helical phases.

It is unlikely that the weak change in spatial parity of

TABLE I.

O_h	(F_1, A_1)	$w^* \text{div}\,\boldsymbol{\xi} + \text{c.c.}$
	(F_1, E)	$\eta_1^*(\partial_x\xi_x + \varepsilon\partial_y\xi_y + \varepsilon^2\partial_z\xi_z) + \eta_2^*(\partial_x\xi_x + \varepsilon^2\partial_y\xi_y + \varepsilon\partial_z\xi_z) + \text{c.c.}$
	(F_2, F_1)	$\eta_x^*(\partial_z\xi_y + \partial_y\xi_z) + \eta_y^*(\partial_x\xi_z + \partial_z\xi_x) + \eta_z^*(\partial_x\xi_y + \partial_y\xi_x) + \text{c.c.}$
	(F_2, A_2)	$\psi^* \text{div}\,\boldsymbol{\zeta} + \text{c.c.}$
	(F_2, E)	$\eta_1^*(\partial_x\zeta_x + \varepsilon\partial_y\zeta_y + \varepsilon^2\partial_z\zeta_z) + \eta_2^*(\partial_x\zeta_x + \varepsilon^2\partial_y\zeta_y + \varepsilon\partial_z\zeta_z) + \text{c.c.}$
D_{6h}	(A_1, E_1)	$\psi^*(\text{rot}\,\boldsymbol{\eta})_z + \text{c.c.}$
	(A_1, A_2)	$\psi^*\partial_z\chi + \text{c.c.}$
	(A_2, E_1)	$\psi^* \text{div}\,\boldsymbol{\eta} + \text{c.c.}$
	(B_1, E_2)	$\psi^*[(\partial_x + i\partial_y)\eta_1 - (\partial_x - i\partial_y)\eta_2] + \text{c.c.}$
	(B_2, E_2)	$\psi^*[(\partial_x + i\partial_y)\eta_1 + (\partial_x - i\partial_y)\eta_2] + \text{c.c.}$
	(B_1, B_2)	$\psi^*\partial_z\chi + \text{c.c.}$
	(E_2, E_1)	$(\xi_1^* + i\xi_2^*)(\partial_x + i\partial_y)\eta_2 + (\xi_1^* - i\xi_2^*)(\partial_x - i\partial_y)\eta_1 + \text{c.c.}$
D_{4h}	(A_1, E)	$\psi^*(\text{rot}\,\boldsymbol{\eta})_z + \text{c.c.}$
	(A_1, A_2)	$\psi^*\partial_z\chi + \text{c.c.}$
	(A_2, E)	$\psi^* \text{div}\,\boldsymbol{\eta} + \text{c.c.}$
	(B_1, E)	$\psi^*(\partial_x\eta_2 + \partial_y\eta_1) + \text{c.c.}$
	(B_2, E)	$\psi^*(\partial_x\eta_1 - \partial_y\eta_2) + \text{c.c.}$
	(B_1, B_2)	$\psi^*\partial_z\chi + \text{c.c.}$

Remark: $\varepsilon = \exp(2\pi i/3)$

UPt_3 (whose confirmation requires further experimental investigation) has quantitative consequences for the superconductivity in this compound. However, with a view to potential applications in the future, in this paper we carry out a detailed investigation of the behavior of the helical phases discovered in Ref. 4 in a magnetic field for a hexagonal crystal without a center of inversion.

According to one currently popular viewpoint, the superconducting state in UPt_3 consists of a mixture of two superconducting states with nearby transition temperatures, belonging to different irreducible representations of the group of point symmetries of the crystal. This makes it possible to explain the observed splitting of the superconducting phase transition in this compound.[5] The representation pairs $(A_{1g}, E_{1g}), (A_{2g}, E_{2g})$, etc. investigated by Joynt et al.[6] all have the same spatial parity—a result of the tacit assumption that inversion symmetry is preserved during the phase transition to the superconducting state. Relaxation of this requirement, i.e., introduction of a new type of unusual superconductivity that breaks the symmetry under spatial inversion of the normal state, can lead to the possibility of helical superconducting phases. In this case, the Lifshits invariants are constructed out of two representations of the group G_0 with opposite parities. A similar method was used by Levanyuk et al.[7] in their study of the problem of phase transitions in certain ferroelectrics.[7]

This paper is structured in the following way. In Sec. 2 we consider helical phases in superconductors that possess a center of inversion, and discuss the applicability of our results to the problem of the splitting of the phase transition in UPt_3. In Sec. 2.1 we classify pairs of representations

out of which Lifshits invariants can be constructed, and discuss the thermodynamics of the helical phases for the example of a mixture of one-dimensional representations A_{1u} and A_{2g} of the group D_{6h}. In Sec. 2.2 we compute the upper critical fields for this system for orientations along the hexagonal axis and in the basal plane. In Sec. 3 we consider helical phases in superconductors without a center of inversion, for the example of the two-dimensional order parameter in UPt_3. Section 3.1 contains an investigation of thermodynamic properties, while in Secs. 3.2 and 3.3 we compute the upper critical fields for helical phases in various field directions relative to the hexagonal axis. Finally, in Sec. 3.4 we investigate the combined effect of the absence of a center of inversion and an orthorhombic deformation.

2. HELICAL PHASES IN SUPERCONDUCTORS WITH A CENTER OF INVERSION

2.1. Ginzburg–Landau functional and helical phases

Let us discuss our general scheme by using a simple example. Assume that the crystal belongs to the hexagonal class. The group D_{6h} has eight one-dimensional (A_1, A_2, B_1, B_2) and four two-dimensional (E_1, E_2) representations with different parities (i.e., with the signs g, u).[8] Assume that the order parameter ψ transforms according to the representation A_{1u} (spin singlet), i.e., $\Delta(\mathbf{k}, \mathbf{r}) = \psi(\mathbf{r})[a\hat{z}k_z + b(\hat{x}k_x + \hat{y}k_y)]$, where $\hat{x}, \hat{y}, \hat{z}$ are unit axial vectors, while the order parameter χ transforms according to the representation A_{2g} (spin triplet), i.e., $\Delta(\mathbf{k}, \mathbf{r}) = \chi(\mathbf{r})[(k_x^3 - 3k_x k_y^2)(k_y^3 - 3k_y k_x^2)]$. Then along with

the usual second- and fourth-order invariants in ψ and χ we can have a cross-term invariant that is linear in the gradient: $\psi^*(d/dz)\chi+$c.c. (here z is along the sixfold axis). The Ginzburg–Landau functional (without a magnetic field) has the following form:

$$\mathscr{F}=\int dV\bigg\{a_1|\psi|^2+a_2|\chi|^2+K_1\bigg|\frac{d\psi}{dz}\bigg|^2+K_2\bigg|\frac{d\chi}{dz}\bigg|^2$$

$$+\beta_1|\psi|^4+\beta_2|\chi|^4+\beta_3|\psi|^2|\chi|^2$$

$$+\beta_4(\psi^{*2}\chi^2+\text{c.c.})+\gamma\bigg(\psi^*\frac{d\chi}{dz}+\text{c.c.}\bigg)\bigg\}, \qquad (1)$$

where $a_{1,2}=\alpha_{1,2}(T-T_{1,2})$ and $K_{1,2}>0$, $\alpha_{1,2}>0$. In general we should also add terms with the gradient in the basal plane. The magnetic field should be introduced in the usual way, i.e., by replacing the gradient with the covariant derivative (see Sec. 2.2 below).

More complicated cases can be treated analogously. In Table I we list the pairs of representations for the groups O_h, D_{6h}, and D_{4h} (i.e., the most interesting groups from the point of view of applications to "heavy fermion" superconductors) out of which it is possible to construct similar invariants. The forms of these invariants are also listed. [It is understood that in each pair the representations are of opposite parity, i.e., for example, (E_2,B_1) implies (E_{2u},B_{1g}) or (E_{2g},B_{1u})]. These pairs satisfy the conditions for the existence of a vector representation in the expansion of their inner product.

Let us now calculate the thermodynamic properties of systems with "Lifshits" invariants. We will use the following modified definitions of the order parameters: $\psi\to\tilde{\psi}=\sqrt{K_1}\psi$, $\chi\to\tilde{\chi}=\sqrt{K_2}\chi$ (the tilde will be omitted in what follows). In order to return to the original units from (1), we must make the following replacements in all the expressions below: $\alpha_{1,2}\to\alpha_{1,2}/K_{1,2}$, $\gamma\to\gamma/\sqrt{K_1K_2}$, $\beta_{1,2}\to\beta_{1,2}/K_{1,2}^2$, and $\beta_{3,4}\to\beta_{3,4}/K_1K_2$. We then write the following Ginzburg–Landau equations obtained from (1) (assuming that $\Delta T=T_1-T_2>0$):

$$-\frac{d^2\psi}{dz^2}+\alpha_1(T-T_1)\psi+\gamma\frac{d\chi}{dz}+2\beta_1|\psi|^2\psi$$

$$+\beta_3|\chi|^2\psi+2\beta_4\chi^2\psi^*=0,$$

$$-\frac{d^2\chi}{dz^2}+\alpha_2(T-T_2)\chi-\gamma\frac{d\psi}{dz}+2\beta_2|\chi|^2\chi \qquad (2)$$

$$+\beta_3|\psi|^2\chi+2\beta_4\psi^2\chi^*=0.$$

The temperature for a phase transition to the superconducting state is determined by the vanishing of the determinant of the linearized system (2). In addition to the trivial solution $\psi=\chi=0$, which describes the normal state, system (2) has uniform and nonuniform solutions of several types, which correspond to various superconducting phases. For example, the solution $\psi,\chi\propto\exp(iqz)$ corresponds to the helical phase (the I phase). The following equation derived from (2) gives the temperature for a transition to this phase:

$$[q^2+\alpha_1(T-T_1)][q^2+\alpha_2(T-T_2)]-\gamma^2q^2=0.$$

The critical temperature T_c is determined by the maximum value of the function $T(q)$ defined above with respect to q. Omitting some rather lengthy operations, we present the results for T_c and q:

$$T_c=\frac{1}{(\alpha_1-\alpha_2)^2}[-\alpha_1\alpha_2(T_1+T_2)+\alpha_1^2T_1+\alpha_2^2T_2$$

$$+\gamma^2(\alpha_1+\alpha_2)-2\gamma^2\sqrt{\alpha_1\alpha_2}\sqrt{d_1}],$$

$$q^2=\tfrac{1}{2}[\gamma^2-\alpha_1(T_c-T_1)-\alpha_2(T_c-T_2)], \qquad (3)$$

where $d_1=1+(\alpha_1-\alpha_2)\Delta T/\gamma^2$.

A phase transition to the helical superconducting phase I takes place for $d_1>0$ and $q^2>0$. Analysis shows that when

$$\Delta T\leqslant(\Delta T)_{c1}=\frac{\gamma^2}{\alpha_2}$$

both these conditions are satisfied, since

$$T_{c1}=T_1+\frac{\alpha_2\gamma^2}{(\alpha_1-\alpha_2)^2}\bigg(\sqrt{d_1}-\sqrt{\frac{\alpha_1}{\alpha_2}}\bigg)^2,$$

$$q^2=-\frac{\alpha_1\alpha_2\gamma^2}{(\alpha_1-\alpha_2)^2}\bigg(\sqrt{d_1}-\sqrt{\frac{\alpha_1}{\alpha_2}}\bigg)\bigg(\sqrt{d_1}-\sqrt{\frac{\alpha_2}{\alpha_1}}\bigg), \qquad (4)$$

(when $\Delta T=\gamma^2/\alpha_2$ we have $T_{c1}=T_1$ and $q=0$). For $\Delta T>(\Delta T)_{c1}$, the helical phase I cannot arise, and a transition takes place from the normal state to a uniform superconducting state with $\psi=\psi_0=\sqrt{\alpha_1(T_1-T)/2\beta_1}$, $\chi=0$ (the II phase) at the temperature T_1. Let us now investigate the stability of this uniform phase II against a helical deformation $\psi=\psi_0+c_1\cos qz$, $\chi=c_2\sin qz$ (phase III). Substituting into the Ginzburg–Landau equation (2) and then linearizing leads to the following equation for the instability temperature (for simplicity we set $\beta_2=\beta_4=0$):

$$[q^2+2\alpha_1(T_1-T)][q^2+\alpha_2(T-T_2)]-\gamma^2q^2=0.$$

The critical temperature T_{c2} and wave vector q are once more determined by maximizing $T(q)$. The results are as follows: For

$$\Delta T>(\Delta T)_{c2}=\gamma^2/2\alpha_1,$$

the helical deformation does not appear; at a temperature $T=T_2$ a phase transition takes place from phase II to another uniform phase $\psi=\psi_0$, $\chi=\chi_0=\sqrt{\alpha_2(T_2-T)/2\beta_2}$ (phase IV). However, if $(\Delta T)_{c1}<\Delta T\leqslant(\Delta T)_{c2}$ holds (which can happen only when $2\alpha_1<\alpha_2$), a transition occurs at the temperature T_{c2} from phase II to the nonuniform phase III, where

$$T_{c2}=T_2+\frac{2\alpha_1\gamma^2}{(2\alpha_1+\alpha_2)^2}\bigg(\sqrt{d_2}-\sqrt{\frac{\alpha_2}{2\alpha_1}}\bigg)^2,$$

$$d_2=\frac{2\alpha_1+\alpha_2}{\gamma^2}\Delta T-1,$$

$$q^2=-\frac{2\alpha_1\alpha_2\gamma^2}{(2\alpha_1+\alpha_2)^2}\bigg(\sqrt{d_2}-\sqrt{\frac{\alpha_2}{2\alpha_1}}\bigg)\bigg(\sqrt{d_2}+\sqrt{\frac{2\alpha_1}{\alpha_2}}\bigg) \qquad (5)$$

(for $\Delta T=\gamma^2/2\alpha_1$ we have $T_{c2}=T_2$ and $q=0$).
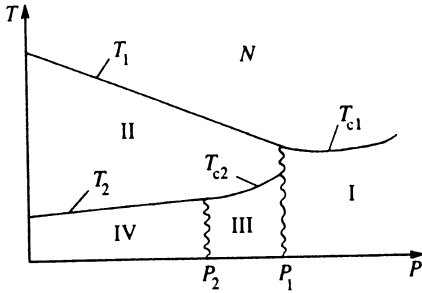
FIG. 1. General form of the phase diagram of a system described by the functional (1). N is the region of the normal state, I–IV are regions of existence of the superconducting phases (for explanation see the text).

Let us now assume that the transition temperatures T_1 and T_2 depend on a parameter (e.g., the pressure P), such that their difference decreases as P increases. Then the phase diagram has the form shown in Fig. 1. The first-order phase transition curves, at which we have $\Delta T(P_1) = (\Delta T)_{c1}$, $\Delta T(P_2) = (\Delta T)_{c2}$, are shown schematically by wavy lines.

Comparing the theoretical phase diagram in Fig. 1 with the experimental data on the behavior of the split superconducting transition of UPt$_3$ as the pressure increases[5] leads us to conclude that the model (1) with two one-dimensional order parameters having differing spatial parities mixed via a Lifshits invariant can provide at least a qualitative explanation for the experimental picture if the condition $\Delta T(P=0) \geqslant (\Delta T)_{c1}$ holds, and if the region where phase III exists disappears (i.e., $2\alpha_1 > \alpha_2$ and the quantity $(\Delta T)_{c1}$ is unobservably small; see Fig. 2). However, we must point out that the first-order phase transition curve shown in Fig. 2 is not observed experimentally; in its place an additional second-order phase transition curve is observed, which must necessarily arise under the assumptions of previous theoretical models.[6,9]

Let us now assume that the condition $\Delta T \leqslant (\Delta T)_{c1}$ is satisfied, so that a transition occurs to the helical phase I as the temperature decreases. There are two possibilities:
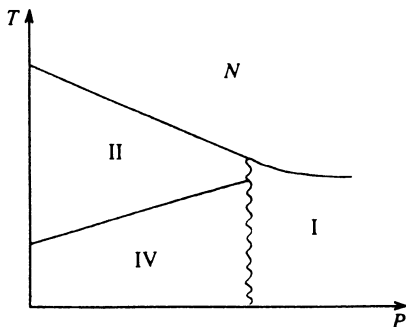

FIG. 2. Phase diagram for special values of the parameters of the problem (see text). The uniaxial pressure P is plotted along the horizontal axis.

(Ia) $\psi = c_1 \cos qz$, $\chi = c_2 \sin qz$,

(Ib) $\psi = c_1 \exp(iqz)$, $\chi = ic_2 \exp(iqz)$. $\qquad$ (6)

The first solution corresponds to a "superconducting cholesteric" phase.

For both phases, the superconducting current $\mathbf{j} = -\delta \mathscr{F}/\delta \mathbf{A}$ equals zero. For the real solution this is immediately obvious, while for the complex solution the absence of a current follows from gauge invariance and the condition that the critical temperature be a maximum (i.e., a minimum of the free energy) as a function of q, i.e., $\delta \mathscr{F}/\delta \mathbf{A} = \delta \mathscr{F}/\delta q = 0$.

In order to choose between phases Ia and Ib, it is necessary to include cubic terms in (2). The corresponding conditions have the following form: for $\tilde{\beta}_2 < \tilde{\beta}_1$, state Ia is realized, while for $\tilde{\beta}_2 > \tilde{\beta}_1$ state Ib is realized (we must add to this the condition of positive definiteness of the fourth-order terms in (1), i.e., $\tilde{\beta}_1 > 0$, $\tilde{\beta}_2 > -\tilde{\beta}_1$), where

$$\tilde{\beta}_1 = \beta_1 + (\beta_2 + \beta_3 - 2\beta_4)k, \qquad \tilde{\beta}_2 = 2\beta_1 + 4\beta_4 k + 2\beta_2 k^2,$$

$$k = \frac{q^2 + \alpha_1(T_c - T_1)}{q^2 + \alpha_2(T_c - T_2)}.$$

As the temperature decreases, the nonlinear terms in the functional distort the cholesteric spiral Ia, and its structure acquires the features of a domain structure: the order parameter is almost uniform over a large portion of each period of the state, and then changes rapidly with a large gradient (a domain wall). At a temperature T_{lock}, a phase transition occurs to a uniform state. Obtaining quantitative information about the nonlinear helical state for $T_{\text{lock}} < T < T_c$ is complicated by the fact that the constant-amplitude approximation that is usually used in the theory of incommensurate phases cannot be used here.[10]

2.2. Magnetic properties of helical phases

Let us consider the behavior of the system described in the previous section in a magnetic field $\mathbf{H}$; that is, let us calculate the upper critical fields for the various superconducting phases. For this, we introduce the following gradient terms in x,y into (1): $K_3|\mathbf{D}\psi|^2 + K_4|\mathbf{D}\chi|^2$, where $D_i = -i\partial_i - A_i$ (we are using units in which $\hbar = 2e = c = 1$ and $h = (2\pi\hbar^2/\Phi_0)H$, where Φ_0 is a flux quantum).

Let the field be directed along the sixfold axis. The temperature $T_{c1}(h)$ of the phase transition from the normal state to the uniform phase II can be found in the standard way, i.e., it is not necessary to take the Lifshits invariant into account. In this case, the Ginzburg–Landau equations decouple and determine the behavior of the two order parameters ψ and χ in the magnetic field independently.

Now let us find $T_{c1}(h)$, i.e., the temperature for a transition from the normal state to the helical phases Ia and Ib. Choosing the gauge $\mathbf{A} = (0, hx, 0)$, we write the linearized Ginzburg–Landau equations as follows:

$$-\frac{\partial^2\psi}{\partial z^2}+K_3h^2x^2\psi-K_3\frac{\partial^2\psi}{\partial x^2}+\alpha_1(T-T_1)\psi+\gamma\frac{\partial\chi}{\partial z}=0,$$

$$-\frac{\partial^2\chi}{\partial z^2}+K_4h^2x^2\chi-K_4\frac{\partial^2\chi}{\partial x^2}+\alpha_2(T-T_2)\chi-\gamma\frac{\partial\psi}{\partial z}=0.$$

$$(7)$$

After the substitution

$$\psi=\exp(iqz)\exp(-(h/2)x^2)\Sigma_n a_n H_n(\sqrt{h}x),$$

$$\chi=\exp(iqz)\exp(-(h/2)x^2)\Sigma_n b_n H_n(\sqrt{h}x),$$

where $H_n(x)$ is a Hermite polynomial, we obtain an algebraic system for a_n and b_n:

$$[\alpha_1(T-T_1)+q^2+2hK_3(n+1/2)]A_n+i\gamma qB_n=0.$$

$$[\alpha_2(T-T_2)+q^2+2hK_4(n+1/2)]B_n-i\gamma qA_n=0.$$

The superconducting transition temperature in a magnetic field is given by the largest zero in n and q of the determinant of this system. We can show that the maximum is reached for $n=0$. The corresponding equation for T_c has the form:

$$[\alpha_1(T-T_1)+q^2+K_3h][\alpha_2(T-T_2)+q^2+K_4h]$$
$$-\gamma^2q^2=0.$$

It is easy to see that finding the transition temperature in a magnetic field reduces to Eq. (3), in which t_1 and T_2 are replaced by

$$T_1\rightarrow T_1-\frac{K_3}{\alpha_1}h,\quad T_2\rightarrow T_2-\frac{K_4}{\alpha_2}h.$$

It is evident that the discussions applying to the previous point remain in force if we consider not the pressure P but the magnetic field h as the parameter on which T_1 and T_2 depend. The phase transition to the helicoidal superconducting phase I in a magnetic field takes place at $q^2>0$, which is the case for

$$\Delta T(h)=T_1-T_2-\left(\frac{K_3}{\alpha_1}-\frac{K_4}{\alpha_2}\right)h<\frac{\gamma^2}{\alpha_2}.$$

Thus, if at $h=0$,

$$T_1-T_2>\frac{\gamma^2}{\alpha_2},$$

then $q=0$, and at the temperature

$$T_1(h)=T_1-\frac{K_3}{\alpha_1}h$$

a transition takes place from the normal state to the superconducting phase II. The corresponding upper critical field is, in dimensional units,

$$H_{c2}(T)=\frac{\Phi_0}{2\pi\hbar^2}\frac{\alpha_1(T_1-T_2)}{K_3}.$$

The difference $\Delta T(h)$ decreases with increase in the field (this takes place at $K_3/\alpha_1>K_4/\alpha_2$) and at the point $\Delta T(h)=(\Delta T_{c1}=\gamma^2/\alpha_2$, the phase transition from the normal state to the superconducting phase II alternates with
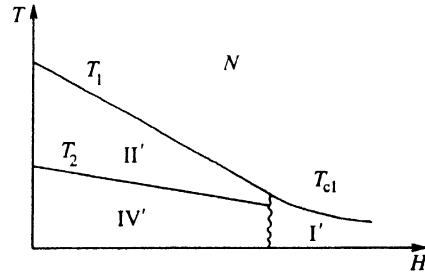

FIG. 3. Phase diagram in a magnetic field. The field H is directed both along the hexagonal axis and in the basal plane. II', IV' are the ordinary Abrikosov vortex phases obtained from the uniform phases II, IV, in a magnetic field; I' is the hexagonal phase I deformed by the magnetic field.

the phase transition of the helicoidal superconducting phase I. The temperature of this transition [see (4)] is

$$T_{c1}(h)=T_{c1}\frac{K_3}{\alpha_1}h+\frac{\alpha_2\gamma^2}{(\alpha_1-\alpha_2)^2}$$

$$\times\left\{\sqrt{1+\frac{\alpha_1-\alpha_2}{\gamma^2}\left[\Delta T-\left(\frac{K_3}{\alpha_1}-\frac{K_4}{\alpha_2}\right)h\right]}-\sqrt{\frac{\alpha_1}{\alpha_2}}\right\}^2.$$

At a temperature below $T_1(h)$, against the background of the already formed mixed state in the superconducting phase II, a phase transition to the superconducting phase IV takes place. The temperature of this transition is determined by the least eigenvalue of the corresponding Ginzburg–Landau equation in a doubly periodic potential that is linear in χ. This potential is given by the spatial distribution of the magnetic field and the order parameter ψ of phase II. It is not possible to find analytically the dependence $T_2(h)$ and to carry out an investigation of phase II on the helicoidal instability (phase III) in a magnetic field. However, there is no doubt of the pressence itself of the phase transition from phase II to phase IV in a magnetic field parallel to the axis of sixth order. Therefore, within the framework of the considered model, the phase diagram of the superconducting phase in a magnetic field along the hexagonal axis, shown in Fig. 3, is possible. Thus, for a mixture of superconducting states, referred to representations of different parity in the field along the hexagonal axis, up to the intersections of the lines $T_1(h)$ and $T_2(h)$, the helicoidal superconducting phase should appear.

If the field is directed into the basis plane or at an arbitrary angle to the axis ε, then the spatial modulation of the superconducting nucleus due to the magnetic field and the Lifshits invariant are no longer independent (as was the case for the field parallel to the c axis). The equations for ψ and χ at $h\neq0$ are not uncoupled. The phase transition from the normal state takes place into the superconducting state, representing its own mixture of the order parameters ψ and χ. Upon further decrease in the temperature, another phase transition takes place into the superconducting phase, which differs from the initial spatial distribution functions ψ and χ. If the lines of these transitions, as functions of the magnetic field, intersect, then the phase

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diagram will coincide qualitatively with the phase diagram of the superconducting phase, constructed from the mixture of representations of the same parity.[6]

Thus, there are important differences of the superconducting states constructed from the mixture of representations with different spatial parity. In this case, for sufficiently small difference of the critical temperatures $\Delta T(P)$ or $\Delta T(\mathbf{H}\| \mathbf{c})$, the superconducting state has a helicoidal structure, the region of existence of which differs from the usual superconducting phases by the lines of phase transition of first order. The given complication makes problematic the explanation of the experimentally established phase diagram of the superconducting phases in UPt within the framework of the considered model.

3. HELICAL PHASES IN SUPERCONDUCTORS WITHOUT A CENTER OF INVERSION

3.1. Helical phases in zero field

As we noted in the Introduction, there are reasons to believe that there is a real violation of spatial parity in UPt$_3$, and that the rotational symmetry is lowered from hexagonal to orthorhombic.

We write the Ginzburg–Landau functional for the two-component order parameter that transforms according to the representation E_1 (or E_2) of the group D_6 (the order parameter has the form $\Delta(\mathbf{k},\mathbf{r}) = \eta_1(\mathbf{r})\phi_1(\mathbf{k}) + \eta2(\mathbf{r})\phi2(\mathbf{k})$, where $\phi_{1,2}$ are basis functions for the corresponding representations[1,2]), taking into account the Lifshits invariant, but neglecting the orthorhombic distortion (the spin state as usual is unimportant):

$$F = \int dV\{\alpha(T-T_0)(|\eta_1|^2+|\eta_2|^2)$$

$$+K_1(D_i^*\eta_j^*)(D_i\eta_j)+K_2(D_i^*\eta_i^*)(D_j\eta_j)$$

$$+K_3(D_i^*\eta_j^*)(D_j\eta_i)+K_4(D_z^*\eta_i^*)(D_z\eta_i)$$

$$+\gamma(\eta_1^*D_z\eta_2-\eta_2^*D_z\eta_1)+\beta_1(|\eta_1|^2+|\eta_2|^2)^2$$

$$+\beta_2|\eta_1^2+\eta_2^2|^2\}, \tag{8}$$

where $i,j=x,y$, $D_j=\nabla_j-i(2e/\hbar c)A_j$ (from here on we will use units in which $\hbar=2e=c=1$). We note that the form of the Lifshits invariant (the term in γ) is the only one possible (i.e., there are no terms that are linear in the gradient with respect to x,y). In order to distinguish effects connected with helical instability, we add to (1) the conditions for magnetic stability formulated in Ref. 11:

$$K_1>|K_3|, \quad K_1+K_2+K_3>|K_2|, \quad K_4>0. \tag{9}$$

Let us begin by investigating the thermodynamic properties of our system in zero magnetic field. Setting $\mathbf{H}=0$ in (8), and assuming the order parameter does not depend on x,y, we obtain the following expression for the free energy density:

$$F=\alpha(T-T_0)(|\eta_1|^2+|\eta_2|^2)+K_4\left(\left|\frac{d\eta_1}{dz}\right|^2+\left|\frac{d\eta_2}{dz}\right|^2\right)$$

$$\times\gamma\left(\eta_1^*\frac{d\eta_2}{dz}-\eta_2^*\frac{d\eta_1}{dz}\right)+\beta_1(|\eta_1|^2+|\eta_2|^2)^2$$

$$+\beta_2|(\boldsymbol{\eta}\boldsymbol{\eta})|^2. \tag{10}$$

The linearized Ginzburg–Landau equations have the form

$$-K_4\frac{d^2\eta_1}{dz^2}+\alpha(T-T_0)\eta_1+\gamma\frac{d\eta_2}{dz}=0,$$

$$-K_4\frac{d^2\eta_2}{dz^2}+\alpha(T-T_0)\eta_2-\gamma\frac{d\eta_1}{dz}=0. \tag{11}$$

In addition to the trivial solution $\eta_1=\eta_2=0$, which describes the normal state, the system (11) has nonzero solutions of two types.

First, the ordinary uniform solutions:

$$\boldsymbol{\eta}=(1,0), \tag{12a}$$

$$\boldsymbol{\eta}=(1,i). \tag{12b}$$

Secondly, the nonuniform solutions:

$$\boldsymbol{\eta}=(c_1\cos qz, c_2\sin qz), \tag{13a}$$

$$\boldsymbol{\eta}=(c_1,ic_2)\exp(iqz), \tag{13b}$$

which describe helical superconducting phases, (13a) real (the "superconducting cholesteric") and (13b) complex.

Again, as in Sec. 2.1, we can show that in the complex helical state the current equals zero due to exact cancellation of the contribution from the usual terms by the contribution from the Lifshits invariant.

The choice between these phases is made by adding terms of fourth order to the free energy. For $\beta_2>0$, the more favorable solution energetically is (13b), while for $\beta_2<0$ it is (13a). The requirement that the fourth-order terms be positive definite also gives the well-known conditions $\beta_1>0$, $\beta_2>-\beta_1$.

The temperature for the transition to the state (12) is T_0. Let us now find the temperature T_c for a transition from the normal state to the helical phase (13), which is determined by setting the determinant of the linear system (11) to zero, which gives $T_c=T_0+\gamma^2/4\alpha K_4$; the wave vector of the structure so obtained is $q=\gamma/2K_4$. The jump in specific heat at this transition for cases (12a) and (13a) is

$$\Delta C=\alpha^2T_c/2(\beta_1+\beta_2),$$

while for cases (12b) and (13b) it is

$$\Delta C=\alpha^2T_c/2\beta_1.$$

As the temperature decreases further, nonlinear distortions in the helical structure toward the real solution (13a) begin to manifest themselves, due to terms of higher order that are omitted in (10). Terms of fourth order cannot fix the phase $\theta(z)$ of the cholesteric spiral $\boldsymbol{\eta}\propto[\cos\theta(z), \sin\theta(z)]$. Therefore it is necessary to consider terms of

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sixth order, one of which, the term $\delta(\eta_+^{*3}\eta_-^3+\eta_-^{*3}\eta_+^3)$, where $\eta_\pm=\eta_1\pm i\eta_2$ fixes the phase at $\theta=\pi/6$ for $\delta>0$ and $\theta=0$ for $\delta<0$.

Substituting the expression for η into the Ginzburg–Landau equation including the sixth-order invariant leads to an equation for $\theta(z)$:

$$K_4\frac{d^2\theta}{dz^2}+\delta|\eta|^4\sin 6\theta=0,$$

i.e., the sine-Gordon equation, as is usual in the theory of incommensurate phases. Repeating well-known arguments [see, e.g., (10)], we have the following results. The components of the order parameter are periodic functions of z with period L (their z-dependence is described by the elliptic sine and cosine; we do not need their exact forms here). With decreasing temperature, the structure acquires the features of a domain structure, i.e., for a large part of the period L the order parameter is almost uniform [a state of type (12a)]; then, over a length $a\sim K_4/\gamma$ that coincides in order of magnitude with the period of the true helical structure for T close to T_c, a rapid transition takes place (a domain wall) between, e.g., $\theta=\pi/6$ and $\theta=2\pi/6$, etc. At a temperature $T_{\text{lock}}<T_c$ a "lock-in" transition occurs to the uniform state (12a).

We emphasize that all this refers only to the real helical state (13a). For the state (13b), the phase is not fixed, and there is no "lock-in" transition.

3.2 Helical phases in a field $H\perp c$

Let us consider the generation of superconducting helicoidal phases in a magnetic field. We limit ourselves to the case of a field directed along a sixth-order axis. After substitution $\eta_{1,2}=\exp(iqz)f_{1,2}(x)$, the Ginzburg–Landau equations take the form

$$(K_1+K_2+K_3)D_x^2f_1+K_1D_y^2f_1+K_2D_xD_yf_2$$

$$+K_3D_yD_xf_2+i\gamma qf_2+(\alpha(T-T_0)+K_4q^2)f_1=0,$$

$$(K_1+K_2+K_3)D_y^2f_2+K_1D_x^2f_2+K_3D_xD_yf_1$$

$$+K_2D_yD_xf_1-i\gamma qf_1+(\alpha(T-T_0)+K_4q^2)f_2=0.$$

For solution of this set we use the method proposed in Ref. 11, namely, we introduce the operators

$$\hat{p}_\pm=\frac{1}{\sqrt{2h}}(D_x\pm iD_y),\quad[\hat{p}_-,\hat{p}_+]=1$$

and the functions

$$f_\pm=\frac{1}{\sqrt{2}}(f_1\pm if_2).$$

The equations are then written down in the form $\hat{A}f=0$, where

$$\hat{A}=\begin{pmatrix} Kh\left(\hat{p}_+\hat{p}_-+\frac{1}{2}\right)-\frac{1}{2}K_-h+ & K_+h\hat{p}_+^2 \\ +\alpha(T-T_0)+K_4q^2+\gamma q & \\ K_+h\hat{p}^2 & Kh\left(\hat{p}_+\hat{p}_-+\frac{1}{2}\right)+\frac{1}{2}K_-h+ \\ & +\alpha(T-T_0)+K_4q^2-\gamma q \end{pmatrix},$$

$$\mathbf{f}=\begin{pmatrix} f_+ \\ f_- \end{pmatrix} \tag{14}$$

and $K=2K_1+K_2+K_3$, $K_\pm=K_1\pm K_2$. We expand $f_\pm$ in eigenfunctions of the operator $\hat{p}_+\hat{p}_-$:

$$f_+\sum_n a_n|n\rangle,\quad f_-=\sum_n b_n|n\rangle.$$

Substituting these expressions in (20), we find that the space of solutions breaks up into a set of independent spaces: 1) $(|0\rangle0)$ and 2) $(a_n|n+2\rangle,b_n|n\rangle$, $n=0,2,4...$. (We consider only the states with even filling numbers n, since states with odd n cannot lay claim to a basic role).

In the first case, we have

$$\alpha(T-T_0)+K_4q^2+\frac{1}{2}(K-K_-)h+\gamma q=0,$$

whence

$$T_c(h)T_0+\frac{\gamma^2}{4\alpha K_4}-\frac{K_1+K_3}{\alpha}h,\quad q=\frac{\gamma}{2K_4}. \tag{15}$$

We now consider the first case. Taking it into account that

$$\hat{p}_+^2|n\rangle=\sqrt{(n+2)(n+1)}|n+2\rangle,$$

$$\hat{p}_|^2|n\rangle=\sqrt{n(n-1)}|n-2\rangle,$$

we obtain an algebraic system for a_n and b_n, from which we obtain

$$\begin{vmatrix} t+Kh\left(n+\frac{5}{2}\right)-\frac{K_-h}{2}+\gamma q & K_+h\sqrt{(n+1)(n+2)} \\ K_+h\sqrt{(n+2)(n+1)} & t+Kh\left(n+\frac{1}{2}\right)+\frac{K_-h}{2}-\gamma q \end{vmatrix}=0, \tag{16}$$

where $t=\alpha(T-T_0)+K_4q^2$. We limit ourselves to the case $n=0$. Then we get the following equation from (16) for the determination of $t(q,h)$:

$$t^2+3tKh+Q=0,$$

where

$$Q=(5K_1^2-2_3^2+7K_1K_2+3K_1K_3-K_2K_3)h^2-\tilde{K}\gamma qh-\gamma^2q^2,$$

$$\tilde{K}=4K_1+K_2+3K_3.$$

The desired solution has the form

$$T(q,h)=T_0-\frac{K_4q^2}{\alpha}-\frac{3Kh-\sqrt{D}}{2\alpha}, \tag{17}$$

where $D=D_04\tilde{K}h\gamma q+4\gamma^2q^2$, $D_0=(8K_+^2+\tilde{K}^2)h^2$. The transition temperature in the magnetic field $T_c(h)$ is de-

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termined by the value of $T(q,h)$ that is maximum in q. The calculations can be carried to completion only in the limiting cases of small and large fields.

As $h \to 0$ we have (with accuracy to second order in h)

$$T_c(h) = T_c + \frac{\gamma^2}{4\alpha K_4} - \frac{K_1 + K_2}{\alpha}h + \frac{2K_4 K_+^2}{\alpha \gamma^2}h^2,$$
$$(18)$$
$$q = \frac{\gamma}{2K_4}\left(1 - \frac{4K_4^2 K_+^2}{\gamma^4}h^2\right).$$

Comparing (15) and (18), we see that the slope of the line $T_c(h)$ is proportional to $-(K_1 + K_3)$ for $K_2 > K_3$ and $-(K_1 + K_2)$ for $K_1 < K_3$. However, in the first case, for increase in the field the situation can become complicated. The introduction of the dependence of q on h for the solution of (18), with increase in the field there appear quadratic corrections to the linear dependence of the transition temperature on h. Therefore, under certain conditions, a kink becomes possible in the line of the upper critical field, which is connected with the intersection of the curve $T_c(h)$ [(18)] and the straight line (15).

In large fields, neglecting the Lifshits invariant, we turn to the results of Refs. 11 and 12 (the helicoidal phase disappears):

$$T_c(h)$$

$$= \begin{cases} T_c - \dfrac{K_1 + K_3}{\alpha}h, & K_- > \dfrac{K_+^2}{K}, \\ T_c - \dfrac{3K - \sqrt{8K_+^2 + (2K - K_-)^2}}{2\alpha}h, & K_- < \dfrac{K_+^2}{K}. \end{cases}$$
$$(19)$$

3.3 Helicoidal phase and orthorhombic deformations

We now consider, along with the absence of a center of inversion, changes in the group G_0 of macroscopic rotational symmetry of the superconductor for which we introduce the tensor of orthorhombic deformations brought about either by interaction with the magnetic moments[9] or by averaging of the noncommensurate density modulations:

$$\varepsilon_{ij} = \begin{pmatrix} u_{xx} & u_{xy} \\ u_{xy} & -u_{yy} \end{pmatrix}.$$

Here, the density of the Ginzburg–Landau functional takes the form

$$F = \alpha(T - T_0)(|\eta_1|^2 + |\eta_2|^2)$$

$$+ K_1(D_i^* \eta_j^*)(D_i \eta_j) + K_2(D_i^* \eta_i^*)(D_j \eta_j)$$

$$+ K_3(D_i^* \eta_j^*)(D_j \eta_i) + K_4(D_z^* \eta_i^*)(D_z \eta_i)$$

$$+ \gamma(\eta_1^* D_z \eta_2 - \eta_2^* D_z \eta_1) + \beta_1(|\eta_1|^2$$

$$+ |\eta_2|^2)^2 \beta_2 |\eta_1^2 + \eta_2^2|^2 + b\varepsilon_{ij}(\eta_i^* \eta_j + \text{c.c.}). \quad (20)$$

We limit ourselves to the study of the thermodynamic properties in zero magnetic field. Setting $D_x \eta = D_y \eta = 0$ in the functional (20), and introducing the notation

$$T_1 = T_0 - \frac{b}{\alpha}u_{xx}, \quad T_2 = T_0 + \frac{b}{\alpha}u_{yy}, \quad \delta = bu_{xy},$$

we obtain the following equation

$$-K_4 \frac{d^2 \eta_1}{dz^2} + \alpha(T - T_1)\eta_1 + \delta \eta_2 + \gamma \frac{d\eta_2}{dz} = 0,$$
$$(21)$$
$$-K_4 \frac{d^2 \eta_2}{dz^2} + \alpha(T - T_2)\eta_2 + \delta \eta_1 - \gamma \frac{d\eta_1}{dz} = 0.$$

The substitution $\eta_{1,2} \propto \exp(iqz)$ reduces the problem to finding the zero of the determinant of the corresponding linear system that is maximum in q:

$$[\alpha(T - T_1) + K_4 q^2][\alpha(T - T_2) + K_4 q^2] - (\gamma^2 q^2 + \delta^2) = 0.$$

We immediately write down the final result

$$T_c = \frac{T_1 + T_2}{2} + \frac{\gamma^2}{4\alpha K_4} + \frac{B^2 K_4}{\alpha \gamma^2},$$
$$(22)$$
$$q^2 = \frac{\gamma^2}{4K_4^2} - \frac{B^2}{\gamma^2},$$

where

$$B^2 = \delta^2 + \frac{1}{4}\alpha^2(T_1 - T_2)^2 = b^2[u_{xy}^2 + \frac{1}{4}(u_{xx} + u_{yy})^2].$$

We note that, in contrast with the situation considered above (Sec. 3.1), the helicoidal instability appears in the described case only at sufficiently high $\gamma : \gamma > \gamma_c = (2BK_4)^{1/2}$. If $\gamma < \gamma_c$, then the transition to the helicoidal phase does not occur and at $\beta_2 > 0$ of the superconducting phase transition will be observed.[9]

The set of equations (21) has solutions of two types [cf. with (13)]: a) $\eta_1 \propto \cos qz$, $\eta_2 \propto \sin qz$—real (cholesteric) and b) $\eta \propto \exp(iqz)$—complex.

Account of fourth order terms yields the result that at $\bar{\beta} > 0$ solution b) prevails, and at $\bar{\beta} < 0$, solution a), where

$$\bar{\beta} = \frac{\alpha^2}{4}(T_1 - T_2)^2(\beta_1 + \beta_2) + \gamma^2 q^2 \beta_2.$$

Quantitative description of the nonlinear distortions, which appear upon decrease in the temperature is difficult, since we cannot apply the approximation of constant amplitude here [see the end of (3.1)]. Nevertheless, it is evident that the picture is qualitatively preserved, i.e., the cholesteric structure becomes similar to a domain one and at some temperature $T_{\text{lock}} < T_c$ a phase transition takes place to the homogeneous state.

4. CONCLUSION

A new type of superconducting state—the helicoidal phase—is of independent interest as a realization of violation of spatial parity C_1 [the latter possibility in the group $G = G_0 \times C_1 \times R \times U(1)$ has not been considered to date]. So far as possible applications to the superconductivity of a known compound, UPt_3, with "heavy fermions" is con-

cerned, a compound in which several superconducting phases are observed, the results of the present investigation do not suggest optimism.

Recent experimental data[3] provide a basis for assuming that UPt$_3$ does not possess macroscopic spatial parity, which allows us to consider the Lifshits invariant in the Ginzburg–Landau functional for the two-component order parameter in standard fashion. Then the splitting of the phase transition could be connected with two successive transitions—the first of second order from the normal to the helicoidal superconducting state and then a weak transition of first order to a homogenous superconducting state. However, the given effect is evidently much too small to be observed.

A second approach has a greater perspective. In this one, the helicoidal phases appear in a spatially even superconductor as a result of a mixture of two order parameters of contrary parity, in this case, on the phase diagrams P-T and H-T (for $H\|$ c, phase transition lines of first order appear in Figs. 2 and 3 that are not observed experimentally). Similar complications, as noted above, also appear in other models.[6] Therefore, the question of the nature of the superconducting state in UPt$_3$ remains open.

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Translated by Frank J. Crowne