Theory of Equilibrium Flux Lattice in UPt_3 under Magnetic Field Parallel to Hexagonal Crystal Axis

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We investigate Abrikosov lattice structures in the unconventional superconductor UPt_3 under magnetic field parallel to the hexagonal crystal axis. Only the two-dimensional E_2 superconducting state among the many other states of different symmetry is compatible with the recent observation [A. Huxley *et al.,* Nature (London) **406**, 160 (2000)] of the flux lattice in the A phase misaligned with crystallographic directions. It is shown that the inequality of the London penetration depths in the basal plane directions resulting from the superposition of hexagonal crystal and superconducting state anisotropies leads for E_2 to a slightly distorted triangular flux lattice.

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It is well accepted that the heavy fermion superconductor UPt_3 exhibits a multicomponent superconducting state. This is obvious when considering the specific phase diagram $H - T$ (magnetic field temperature) for the mixed state (see Fig. 1). This diagram clearly shows three distinct superconducting phases: A, B, and C [1–3]. The theoretical models that have been proposed to explain the phase diagram belong to two main categories. In the first class of theories, the zero-field phase transition splitting is due to the lifting of the degeneracy between the components of one multicomponent superconducting state [4–6]. This lifting results from the action of a symmetry breaking field which is presumably connected with antiferromagnetic ordering of tiny magnetic moments located on uranium atoms [7–9]. The other sources of the symmetry breaking field that have been discussed are (i) the small crystal field anisotropy or spin orbital interaction [10–12] and (ii) the possible incommensurate modulations of the crystal density [13]. The second type of multicomponent treatment of the phase diagram is given in [14], where the phase transition splitting is deduced from the existence of two one-component superconducting states of different symmetry with accidentally close critical temperatures. One of the two states corresponds to the A phase, the other to the C phase, and the mixture of both to the B phase.

The recent comprehensive analysis of the thermodynamic and transport data presented in the paper [15] says in favor of the two-dimensional (2D) spin-triplet E_{2u} superconducting state with the particular angular dependence of the pairing interaction proposed in [16] as a development of the initial model [4]. The achievement of the correspondence between a microscopic theory and the experiments each time implies some specific model assumptions. That is why the direct experimental manifestations of the symmetry of the superconducting states are desirable for the unambiguous identification of phases. Such an experiment—the small angle neutron scattering with the direction of magnetic field parallel to the hexagonal axis of UPt_3—has been performed recently in Grenoble [17] for A and B phases.

In the A phase of UPt_3, an unusual alignment of the Abrikosov lattice rotated over $\pm 15°$ from the **a** crystallographic direction was discovered. On the contrary, in the B phase the flux lines lattice (FLL) orientation did not reveal a misalignment with hexagonal directions (see the details of the experimental performance in [17]). In both A and B phases, the flux lattices were close to the perfect hexagonal. These observations were interpreted by the authors of [17] as the proof of the identification of A and B phases with a superconducting state corresponding to the 2D E_{2u} model. Being accordant with this statement, we have to note that it was done on the basis of the London approach with the lowest order nonlocal correction developed for the case of conventional [18] and nonconventional [19] 1D superconducting states. The corresponding theory for the 2D superconductivity has its own peculiarities, so our aim is to develop the proper description of the equilibrium FLL

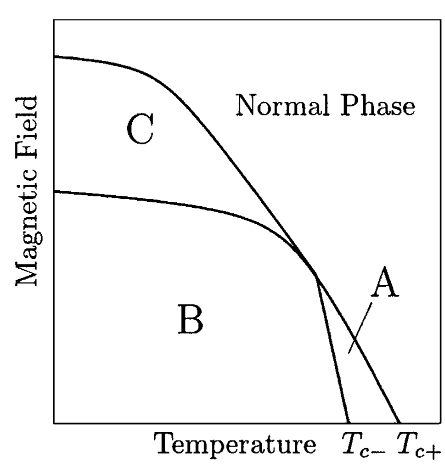

FIG. 1. Schematic phase diagram of the superconducting mixed state of UPt_3 for magnetic fields parallel to the hexagonal crystal axis.

structures for the 2D superconducting states in hexagonal crystals with the magnetic field parallel to the crystal axis. The earlier UPt_3 FLL scattering experiments [20,21] and the theory of the equilibrium FLL [22] were related to the basal plane orientation of the magnetic field.

In this Letter, we show that, for the field parallel to the c axis, (i) the Abrikosov lattice orientation is fixed by general symmetry considerations, and (ii) the distortion of the Abrikosov unit cell can be partly found in the frame of the London local approximation. The latter is a unique property of 2D superconductivity in the uniaxial crystals where, unlike 1D superconductivity, the basal plane anisotropy of the tensor of superfluid density occurs. As a result, the A phase FLL for the E_{1g} superconducting state must be strongly distorted and aligned with the hexagonal basal plane crystallographic directions. On the contrary, the slightly distorted hexagonal FLL rotated over the angles $\approx \pm 15°$ from the crystal $\mathbf{a}$ direction observed in the A phase of UPt_3 corresponds to the 2D E_{2u} superconducting state.

When the magnetic field is oriented along the hexagonal axis, there are only two sources for the basal plane anisotropy: the sixfold anisotropy of the crystal itself and the possible anisotropy of the unconventional superconducting state or, more explicitly, the directional dependence of the modulus of the gap function in the $\mathbf{k}$ space determining the expression for the superconducting currents in the London electrodynamics. For any 1D superconducting state in the hexagonal crystal with strong spin-orbital coupling, this symmetry coincides with the hexagonal symmetry of the crystal [23]. That is why there are no preferential directions in the basal plane besides $\mathbf{a}$, $\mathbf{a}^*$, and the directions rotated with respect to them over the angles $n\pi/3$, $n = 1, 2$. In this case, there is no reason for the A-phase misalignment of the FLL. Therefore we need to consider only 2D superconducting states. We shall limit ourselves to the most popular singlet E_{1g} and triplet E_{2u} states.

In the even-parity model E_{1g}, the superconducting state is described by a complex 2D vector $\boldsymbol{\eta} = (\eta_1, \eta_2)$. The gap function is $\Delta^{E_{1g}}{}_{\mathbf{k}}(\mathbf{r}) = \cos\theta \sin\theta[\eta_1(\mathbf{r}, T) \times \cos\varphi + \eta_2(\mathbf{r}, T)\sin\varphi]$. Here, φ and θ, are, respectively, the azimuthal (in the basal plane) and polar angles of the relative momentum of the particles in the Cooper pair related to crystal axes. A complex two-component order parameter $\boldsymbol{\eta} = (\eta_1, \eta_2)$ is also considered in the E_{2u} model, where the orbital gap function has the form $\Delta^{E_{2u}}{}_{\mathbf{k}}(\mathbf{r}) = \hat{\mathbf{z}} \cos\theta \sin^2\theta[\eta_1(\mathbf{r}, T)\cos 2\varphi + \eta_2(\mathbf{r}, T)\sin 2\varphi]$.

At zero field, the order parameter is identified with $\boldsymbol{\eta} = (1, 0)$ in the A phase and with $\boldsymbol{\eta} = [1, ib(T)]$ in the B phase, where $b(T)$ is a decreasing function with temperature which gets to zero at T_{c-}. It is commonly believed that the phase transition splitting results from an antiferromagnetic (AF) symmetry breaking field which acts in favor of one of the two components of the superconducting state. Actually, there are three types of AF domains with different orientations of staggered magnetization [24]. One can see, however, that the two types of three differently oriented domains act in favor of the same component of the superconducting order parameter. The third type of domain acts in favor of the other component. Its appearance shall create additional inhomogeneities on the boundaries between domains. In view of more or less close sizes of the AF domains and of the A phase superconducting coherence length, the inhomogeneous superconducting state seems to be energetically nonprofitable in comparison with a one-component homogeneous superconducting state in the whole specimen's volume. That is why we shall make our derivation in the frame of a single domain picture of the symmetry breaking field causing, first, the appearance of one definite component of a 2D superconducting state in the whole specimen's volume.

Under magnetic field in the A and B phases, both components of $\boldsymbol{\eta}$ coexist and depend on space coordinates. We can claim, however, that in the A phase the second component in the vicinity of the upper critical temperature $T \approx T_{c+}$ is much smaller than the first one: $|\eta_2| \ll |\eta_1|$. Indeed, in the A phase (η_1, η_2) are related via the Ginzburg-Landau equations as (see, for example, Ref. [23])

$$(K_{123}D_x^2 + K_1 D_y^2)\eta_1 + (K_2 D_x D_y + K_3 D_y D_x)\eta_2 + \alpha_0 \tau_1 \eta_1 = 0, \tag{1}$$

$$(K_{123}D_y^2 + K_1 D_x^2)\eta_2 + (K_3 D_x D_y + K_2 D_y D_x)\eta_1 + \alpha_0 \tau_2 \eta_2 = 0, \tag{2}$$

where $\tau_1 = (T - T_{c+})/T_{c+} < 0$, $\tau_2 = (T - T_{c-})/T_{c-} > 0$, $K_{123} = K_1 + K_2 + K_3$, $D_i = -i\nabla_i + 2\pi A_i/\phi_0$ (here, ϕ_0 is the magnetic flux quantum and $\mathbf{A}$ is the vector potential), and the coefficients K_1, K_2, K_3, and α_0 are positive constants. Neglecting the terms containing the differential operators acting on η_2 (which is justified by the result), we solve first Eq. (1). By substituting the result in Eq. (2), we get

$$\eta_2 \sim i \frac{K_2 + K_3}{\sqrt{K_{123}K_1}} \frac{|\tau_1|}{|\tau_2|} \eta_1 . \tag{3}$$

As long as $|\tau_1| \ll |\tau_2|$, we have $|\eta_2| \ll |\eta_1|$. For the E_{2u} superconducting state, the latter property takes place in the whole region of existence of the A phase in view of the inequality $K_2 + K_3 \ll K_1$ specific for this state [16] (see also below).

So, one can say that in the A phase we have an additional source of anisotropy which roughly corresponds to the symmetry of the modulus of the gap function of the two-component superconducting state. This symmetry is determined by the symmetry of the functions $|\eta_1 \cos\varphi + \eta_2 \sin\varphi|$ for the E_{1g} state and $|\eta_1 \cos 2\varphi + \eta_2 \sin 2\varphi|$ for the E_{2u} state. The first function has only (xz) and (yz) planes as symmetry planes passing through the hexagonal crystal axis. The second function has two additional planes of symmetry obtained from the former ones by rotations over the angles $\pm 45°$ around the z axis (bisecting planes). This means that the E_{1g} superconducting state does not create a basal plane anisotropy corresponding to the A phase FLL orientations rotated over $\pm 45°$ with respect to the basal plane hexagonal crystal directions. On the contrary, such an anisotropy definitely exists in the superconducting E_{2u} state. In presence of a small hexagonal anisotropy, the FLL configurations must be weakly deviated from $\pm 45°$ since the bisecting planes are not symmetry planes for the Fermi surface. The weights of the components of the order parameter in the superconducting B phase are approximately equal so that they effectively recreate the basal plane isotropy and eliminate the reason for misalignment of the vortex lattice with respect to the crystal directions.

If the FLL orientations could be established on a pure symmetry basis, the finding of the lattice distortions requires more quantitative considerations. UPt_3 is a strong type-II superconductor with a Ginzburg-Landau parameter $\kappa \approx 60$: It means that the London local and linear electrodynamic description is valid for any temperature and magnetic field $H \ll H_{c2}$. The experiment [17] has been performed at a much higher field $H \approx 0.4 H_{c2}$. However, for simplicity, we shall discuss the equilibrium shape of the FLL in the frame of the London approach. Then we shall demonstrate the coincidence of the London equilibrium configurations to those which are established in the Ginzburg-Landau approximation valid for higher fields $H \approx H_{c2}$.

In the London theory, the Fourier components of the superconducting current density $\mathbf{j}(\mathbf{q})$ and the vector potential $\mathbf{A}(\mathbf{q})$ are related via

$$j_i(\mathbf{q}) = -\frac{c}{4\pi} Q_{ij}(\mathbf{q}) A_j(\mathbf{q}) . \qquad (4)$$

In the clean limit, the electromagnetic response tensor $Q_{ij}(\mathbf{q})$ has been pointed out for the arbitrary superconducting state and arbitrary Fermi surfaces [19]:

$$Q_{ij}(\mathbf{q}) = \frac{4\pi T}{\lambda_0^2} \sum_{n>0} \left\langle \frac{|\Delta_{\hat{\mathbf{k}}}|^2 \hat{v}_{Fi} \hat{v}_{Fj}}{\sqrt{\omega_n^2 + |\Delta_{\hat{\mathbf{k}}}|^2} (\omega_n^2 + |\Delta_{\hat{\mathbf{k}}}|^2 + \gamma_{\mathbf{q}}^2)} \right\rangle , \qquad (5)$$

where $\boldsymbol{v}_F$ is the Fermi velocity and $\hat{v}_{Fi} = v_{Fi}/v_F$, $\gamma_{\mathbf{q}} = \boldsymbol{v}_F \cdot \mathbf{q}/2$, $\omega_n = \pi(2n-1)T$ are Matsubara frequencies, λ_0 is the London penetration depth at $T = 0$, and the angular brackets mean the average over the Fermi surface.

The equilibrium vortex lattice minimizes the free energy density [18] at a given magnetic induction $\mathbf{B}$:

$$F = \frac{B^2}{8\pi} \sum_{\mathbf{q}=\mathbf{G}} f(\mathbf{q}) , \qquad (6)$$

where the sum extends over all reciprocal lattice vectors $\mathbf{G}$ and

$$f(\mathbf{q}) = \frac{g(\mathbf{q})}{1 + q_x^2 (Q^{-1})_{yy} + q_y^2 (Q^{-1})_{xx} - q_x q_y [(Q^{-1})_{xy} + (Q^{-1})_{yx}]} . \qquad (7)$$

The cutoff factor $g(\mathbf{q})$ corrects the failure of the London approximation in the vortex cores.

We need now to calculate the electromagnetic response tensor $Q_{ij}(\mathbf{q})$. It is developed in powers of the quantity $\gamma_{\mathbf{q}}^2$: $Q = Q^{(0)} + Q^{(2)} + \ldots$, where $Q^{(0)} \ll Q^{(2)}$. At leading order, which corresponds to the London local approximation, we have

$$f(\mathbf{q}) = \frac{g(\mathbf{q})}{1 + \lambda^2 [q^2 + c_1 (q_x^2 - q_y^2) + 2 c_2 q_x q_y]} , \qquad (8)$$

where $\lambda^2 = (Q_{xx}^{(0)} + Q_{yy}^{(0)})/2 \det Q^{(0)}$, $c_1 = (Q_{xx}^{(0)} - Q_{yy}^{(0)})/(Q_{xx}^{(0)} + Q_{yy}^{(0)})$, and $c_2 = 2 Q_{xy}^{(0)}/(Q_{xx}^{(0)} + Q_{yy}^{(0)})$.

The dimensionless coefficients c_μ originate from the anisotropies of the Fermi surface and the superconducting gap. They are nonzero only for the 2D superconducting states. Since in the A phase we are in the Ginzburg-Landau region, the gap function in the denominator of (5) can be neglected and the coefficients giving the anisotropic terms are expressed as

$$c_1 \sim \frac{\langle |\Delta_{\hat{\mathbf{k}}}|^2 (\hat{v}_{Fx}^2 - \hat{v}_{Fy}^2) \rangle}{\langle |\Delta_{\hat{\mathbf{k}}}|^2 \rangle} , \qquad c_2 \sim \frac{\langle |\Delta_{\hat{\mathbf{k}}}|^2 2 \hat{v}_{Fx} \hat{v}_{Fy} \rangle}{\langle |\Delta_{\hat{\mathbf{k}}}|^2 \rangle} . \qquad (9)$$

In order to evaluate the averages over the Fermi surface, we consider for simplicity a cylindric energy spectrum with a weak in-plane hexagonal anisotropy [16]:

$$\epsilon_{\mathbf{k}} = (\hbar^2/2m_\perp)(k_x^2 + k_y^2) + 2a\epsilon_F \cos 6\varphi . \qquad (10)$$

Here, ϵ_F is the Fermi energy and $a \ll 1$. Therefore the average is expressed as $\langle \ldots \rangle = \int_0^{2\pi} d\varphi (1 - a\cos 6\varphi)(\ldots)/2\pi$, and the velocity at the Fermi surface at first order in a becomes

$$\hat{v}_{Fx} = \cos\varphi + 3a(\cos 5\varphi - \cos 7\varphi) , \qquad (11)$$

$$\hat{v}_{Fy} = \sin\varphi - 3a(\sin 5\varphi + \sin 7\varphi) . \qquad (12)$$

We find for E_{1g}:

$$c_1 = \frac{1}{2} \frac{|\eta_1|^2 - |\eta_2|^2}{|\eta_1|^2 + |\eta_2|^2} , \qquad c_2 = \frac{\Re(\eta_1 \eta_2^*)}{|\eta_1|^2 + |\eta_2|^2} , \qquad (13)$$

and for E_{2u}:

$$c_1 = \frac{11}{4} a \frac{|\eta_1|^2 - |\eta_2|^2}{|\eta_1|^2 + |\eta_2|^2} ,$$

$$c_2 = -\frac{11}{2} a \frac{\Re(\eta_1 \eta_2^*)}{|\eta_1|^2 + |\eta_2|^2} . \qquad (14)$$

Since after Eq. (3) $\Re(\eta_1 \eta_2^*) = 0$ in the A phase, only the anisotropic term with the coefficient c_1 exists in the A phase. The effect of such an anisotropy has been studied by Kogan [25].

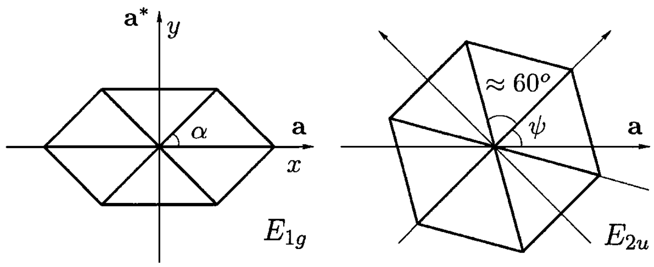

FIG. 2. One vortex lattice configuration for both superconducting states E_{1g} and E_{2u}. The E_{1g} state yields a square FLL (with $\alpha \approx 45°$) aligned with crystallographic directions. In the E_{2u} state, the FLL is almost perfectly hexagonal and oriented along directions at $\psi \approx \pm 45°$ with regard to the **a** crystallographic axis.

Following [18,25] we shall consider the vortex lattice configurations symmetric with regard to reflections by (xz) and (yz) planes for E_{1g} state. There are two possible distorted FLL [25]. In the first configuration, the angle of distortion α between the two basis vectors of the unit cell of the FLL is given for $H \gg H_{c1}$ by

$$\tan\alpha = \sqrt{3}\left(\frac{Q_{yy}^{(0)}}{Q_{xx}^{(0)}}\right)^{1/2} = \sqrt{3}\left(\frac{1 - c_1}{1 + c_1}\right)^{1/2}. \qquad (15)$$

For $|\eta_2| \ll |\eta_1|$, the E_{1g} state therefore predicts a strong distortion with $\alpha \approx 45°$ (a square FLL, see Fig. 2). The value of α depends on the form of the energy spectrum. For the second configuration, the FLL is also strongly distorted.

For the E_{2u} state, the FLL configurations rotated over the angles $\pm 45°$ can be obtained by the same procedure as for E_{1g} only at $a = 0$ when the bisecting planes are planes of symmetry for the FLL. In this case, $c_1 = c_2 = 0$ and the FLL has the perfect hexagonal structure. In the presence of a small hexagonal anisotropy, the FLL configuration is both slightly distorted ($\sim a$) and oriented at $\psi \approx \pm 45°$ (Fig. 2).

The application of Abrikosov-type formalism developed in Ref. [26] for the ordinary superconductors with effective mass anisotropy leads to the same conclusions. To see this, one needs to take into account the property $|\eta_1| \gg |\eta_2|$ to consider the Ginzburg-Landau Eq. (1) only for η_1. Then remembering that $(K_2 + K_3) \sim K_1$ for the E_{1g} superconducting state and $(K_2 + K_3) \sim aK_1$ for the E_{2u} superconducting state (see [16]), we come to the statement formulated above.

In conclusion, we have described theoretically the orientations and the distortions of the flux lattice in the superconducting A phase of UPt_3 considering all possible superconducting states of different symmetry. Only the E_{2u} state is consistent with the recently observed [17] specially oriented and almost perfectly hexagonal vortex lattice configuration. This statement and the theoretical description of the low temperature behavior of the thermodynamic and transport properties [15] definitely settle the two-component E_{2u} superconducting state in UPt_3.

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