# Model of isotropic *d*-wave pairing in $UPt_3$

M. E. Zhitomirskiĭ and I. A. Luk'yanchuk
*L. D. Landau Institute of Theoretical Physics, Russian Academy of Sciences, 117 334, Moscow*

(Submitted 23 June 1993)
Pis'ma Zh. Eksp. Teor. Fiz. **58**, No. 2, 127–133 (25 July 1993)

A phenomenological model is proposed for describing the *H–T–P* phase diagram of the heavy-fermion superconductor $UPt_3$. In this model, the $UPt_3$ is a nearly isotropic *d*-wave superconductor whose transition temperature is split slightly by the crystal field. This model agrees with all known experimental data on the phase diagram of $UPt_3$. The parameter values used are close to those predicted by weak-coupling theory. Physical reasons for such isotropy of superconducting properties are discussed.

A splitting of the superconducting transition in the compound $UPt_3$ was discovered about five years ago.[1] It is one of the major pieces of evidence for a nontrivial pairing of electrons in several heavy-fermion superconductors. The reason for this splitting, on the other hand, is not yet clear. None of the existing phenomenological models[2–4] can completely explain the experimental data available: the splitting of $T_c$, the kink on the $H_{c2}(T)$ curve for all directions of the magnetic field, and the *H–T–P* phase diagram.[5]

In this letter we offer a model from which all known experimental results follow in a natural way. This model is based on some recent studies of the $UPt_3$ crystal structure.[6,7] Some ABACABAC...stacking faults were found in the *hcp* lattice of uranium atoms (ABAB...). These faults correspond to a double hexagonal structure. The presence of such defects is often evidence that the crystal is close to a transition to an fcc structure.[8] The size of these defects, $a \sim 30$ Å (Ref. 6), is smaller than the coherence length $\xi_0 \sim 150$ Å. The existence of these defects should thus cause the spectrum of excitations responsible for the formation of Cooper pairs to tend toward isotropy.

We accordingly suggest that the pairing of electrons in $UPt_3$ with a relative angular momentum $l=2$ occurs in nearly isotropic surroundings. The lower symmetry of the crystal lattice causes only a slight splitting of the transition temperature of a fivefold-degenerate *d* multiplet. A similar model for *p*-wave pairing was studied in Ref. 9, but that model did not predict the kink on the $H_{c2}(T)$ curve for magnetic fields in the basal plane of the crystal.

Our analysis starts from the $SO(3)$-symmetry Ginzburg–Landau functional for a singlet superconducting order parameter $\Delta(\mathbf{k}) = \Sigma a_m Y_{2m}(\mathbf{k}/|\mathbf{k}|) = B_{ij}k_ik_j$ ($\mathbf{k}$ is the momentum on the Fermi surface, $Y_{2m}$ are the second-order spherical harmonics, and $\mathrm{Tr}B=0$):

  

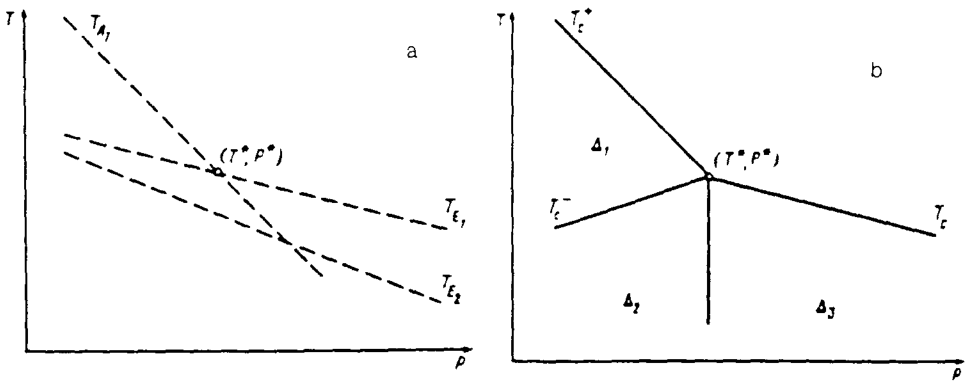


FIG. 1. a—Splitting of the transition temperature for isotropic $d$-wave pairing caused by a crystal field with symmetry $D_6$; b—phase diagram of $UPt_3$ at $H=0$.

$$F=\alpha(T-T_c)\mathrm{Tr}B^*B+\beta_1(\mathrm{Tr}B^*B)^2+\beta_2|\mathrm{Tr}B^2|^2+\beta_3\mathrm{Tr}(B^{*2}B^2)$$

$$+K_1\nabla_i^*B_{jk}^*\nabla_iB_{jk}+K_2\nabla_i^*B_{ik}^*\nabla_jB_{jk}+K_3\nabla_i^*B_{jk}^*\nabla_jB_{ik},\quad \nabla_i=\partial_i-i\frac{2e}{\hbar c}A_i. \tag{1}$$

In weak-coupling theory we would have $\beta_2=0.5\beta_1$, $\beta_3=0$, and $K_2=K_3=2K_1$. It was shown in Ref. 10 that under the condition $\beta_2>0$ the following states prevail, depending on the sign of $\beta_3$:

$$\begin{aligned}&\Delta(\mathbf{k})\sim(k_x+ik_y)^2, && \beta_3>0,\\ &\Delta(\mathbf{k})\sim k_x^2+e^{2\pi i/3}k_y^2+e^{4\pi i/3}k_z^2, && \beta_3<0.\end{aligned} \tag{2}$$

The case $\beta_3=0$ is degenerate: Any matrix $B$ satisfying $\mathrm{Tr}B^3=0$ minimizes functional (1). Another mechanism for a lifting of this degeneracy is a splitting of $T_c$. The crystal field splits the transition temperature for pairing with $l=2$ in accordance with the three irreducible representations of the $D_6$ group:

$$\Delta(\mathbf{k})\sim k_x^2+k_y^2-2k_z^2 \quad -A_1,$$

$$\Delta(\mathbf{k})\sim(k_x\pm ik_y)k_z \quad -E_1,$$

$$\Delta(\mathbf{k})\sim(k_x\pm ik_y)^2 \quad -E_2. \tag{3}$$

The direction of $\hat{z}$ is along the sixfold rotation axis, while $\hat{x}$ and $\hat{y}$ lie in the basal plane of the crystal.

We are thus suggesting that the effect which primarily determines the structure of the phase diagram is the splitting of the transition temperature for $d$-wave pairing. We ignore the effect of the crystal field on the fourth-degree terms and on the inhomogeneity energy in (1).

## P–T PHASE DIAGRAM

Symmetry arguments place no restrictions on the relations among the transition temperatures for representations (3). These temperatures should depend on the pressure, and even small deformations of the lattice can change their order. An analysis of all possible cases reveals that the $UPt_3$ phase diagram can be explained with the single arrangement of transition temperatures in the $P$–$T$ plane shown in Fig. 1a. The polycritical point $(P^*,T^*)$ is determined by the intersection of lines $T_{A1}(P)$ and $T_{E1}(P)$, which correspond to phase transitions involving irreducible representations $A_1$ and $E_1$. An applied pressure thus "restores" the isotropy, and at $P=P^*$ the splitting effect of the crystal field is particularly weak.

To study the phase diagram we need to consider fourth-degree terms. Representation $E_2$ can be ignored near the polycritical point. Expanding the order parameter in basis functions of the two other representations, we find, in place of (1),

$$F=\alpha(T-T_{A1})|a_0|^2+\alpha(T-T_{E1})(|a_1|^2+|a_{-1}|^2)$$
$$+\beta_1(|a_0|^2+|a_1|^2+|a_{-1}|^2)^2+\beta_2|a_0^2+2a_1a_{-1}|^2. \qquad (4)$$

We have discarded a term with $\beta_3$ from (4). This is legitimate since the degeneracy which prevailed in the case $\beta_3=0$ is now lifted by the splitting of $T_c$; although the coefficient $\beta_3$ is not zero, it is generally small if strong-coupling effects are small.

At pressures below $P^*$ a superconducting transition occurs at the temperature $T_c^+=T_{A1}$ to the phase

$$\Delta_1(\mathbf{k})=\frac{a_0}{\sqrt{6}}(k_x^2+k_y^2-2k_z^2),\quad a_0^2=\frac{\alpha(T_{A1}-T)}{2(\beta_1+\beta_2)}. \qquad (5)$$

Only the gauge symmetry of the system is broken in the process. Solution $\Delta_1(\mathbf{k})$ is invariant under the group $D_6\times R$. The next phase transition occurs at $T=T_c^-$:

$$T_c^-=\frac{1}{2}\left[T_{A1}\left(1-\frac{\beta_1}{\beta_2}\right)+T_{E1}\left(1+\frac{\beta_1}{\beta_2}\right)\right]. \qquad (6)$$

Below $T_c^-$ the minimum energy corresponds to the phase

$$\Delta_2(\mathbf{k})=\frac{a_0}{\sqrt{6}}(k_x^2+k_y^2-2k_z^2)+\sqrt{2}a_1ik_xk_z,$$

$$a_1^2=\frac{\alpha(T_c^--T)}{4\beta_1},\quad a_0^2=a_1^2+\frac{\alpha(T_{A1}-T_{E1})}{4\beta_2}. \qquad (7)$$

The symmetry of the $\Delta_2(\mathbf{k})$ phase is $D_2(U_{2y})$. For the ratio of jumps in the specific heat we find the standard expression:

$$\frac{\delta(C/T)(T_c^-)}{\delta(C/T)(T_c^+)}=\frac{\beta_2}{\beta_1}. \qquad (8)$$

At $P>P^*$, there is only the one phase transition, at $T_c=T_{E1}$, to the phase

$$\Delta_3(\mathbf{k}) = a_1(k_x + ik_y)k_z, \quad a_1^2 = \frac{\alpha(T_c - T)}{2\beta_1}, \tag{9}$$

which corresponds to symmetry group $D_6(E)$. Since $D_2(U_{2y}) \not\subset D_6(E)$, a vertical line of second-order transitions lies between the $\Delta_2(\mathbf{k})$ and $\Delta_3(\mathbf{k})$ phases on the $P$–$T$ diagram (it is vertical if the coefficient $\beta_3$ is ignored). There is an abrupt change in the volume (or length) of the sample at this line:

$$\frac{\delta V}{V} = \frac{\alpha^2(T^* - T)}{4\beta_1}\left(\frac{\partial T_{A1}}{\partial P} - \frac{\partial T_{E1}}{\partial P}\right). \tag{10}$$

If this jump were to be observed, in anomalies in elastic properties, for example, it might prove a decisive argument in favor of the model proposed here. The resulting phase diagram is shown in Fig. 1b.

The symmetry of the $\Delta_2(\mathbf{k})$ phase allows a continuously variable admixture of components of the $E_2$ representation. Γhis admixture begins directly at the temperature $T_c^-$. Accordingly, when the sample is cooled to the transition temperature $T_{E2}(P)$, there is no additional phase transition associated with representation $E_2$. Instead, an anomaly in the specific heat should appear, with a relative size on the order of $\beta_3/\beta_1$; this anomaly should be broadened and become diffuse along the temperature scale. [The admixture of $E_2$ components arises because of the term with $\beta_3$ in energy functional (1).]

A nonzero $\beta_3$ makes the phases $\Delta_2(\mathbf{k})$ and $\Delta_3(\mathbf{k})$ unfavorable in comparison with one of the phases in (2) from the energy standpoint in a case in which we can ignore the splitting of $T_c$. Under the condition $|\beta_3| \leqslant (T_{E1} - T_{E2})/T_{E1}$, however, this situation does not arise down to extremely low temperatures.

## *H–T* PHASE DIAGRAM

We can now show that a kink on the $H_{c2}(T)$ curve should occur for both $\mathbf{H} \perp \hat{z}$ and $\mathbf{H} \parallel \hat{z}$. We take a symmetry approach,[11] assigning various quantum numbers to the vortex lattices near $H_{c2}$.

In the case $\mathbf{H} \parallel \hat{z}$ the gradient energy for the $A_1$ and $E_1$ representations found from (1) is

$$F_{\text{grad}} = \left(K_1 + \frac{1}{4}K_{23}\right)|\nabla_i a_{\pm 1}|^2 - \frac{1}{4}K_{23}(a_{-1}^*\nabla_+^2 a_{+1} + a_{+1}^*\nabla_-^2 a_{-1})$$
$$-\frac{eH}{2\hbar c}\tilde{K}_{23}(|a_{+1}|^2 - |a_{-1}|^2) + \left(K_1 + \frac{1}{6}K_{23}\right)|\nabla_i a_0|^2. \tag{11}$$

Here we have set $\nabla_z a_m = 0$, $\nabla_\pm = \nabla_x \pm i\nabla_y$, $K_{23} = K_2 + K_3$, and $K_{23} = \tilde{K}_2 - K_3$.

The critical field is at a maximum for the following solutions of the linearized Ginzburg–Landau equations:

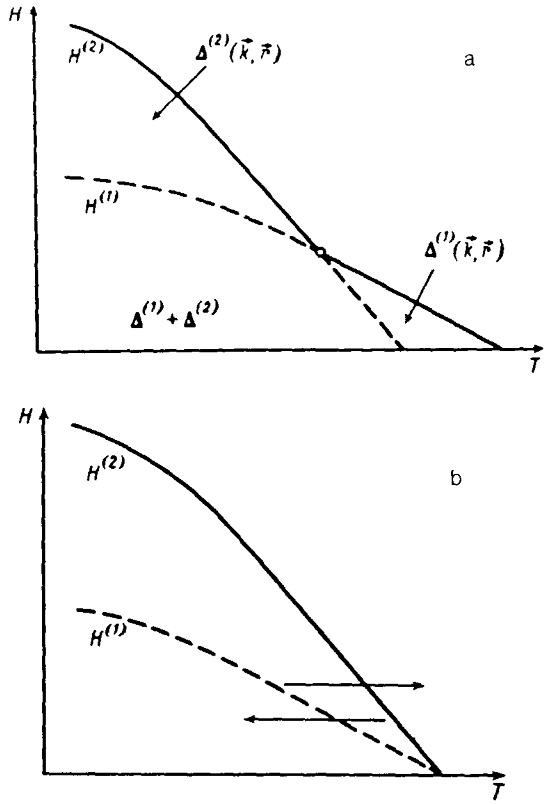


FIG. 2. a—Critical fields and superconducting phases in the case $\mathbf{H} \parallel \hat{z}$, $P<P^*$ (in the case $\mathbf{H} \perp \hat{z}$, the phase diagram has a similar structure); b—critical fields for isotropic $d$-wave pairing. The arrows show the splitting of the $H^{(1)}(T)$ and $H^{(2)}(T)$ branches by crystal field at $P<P^*$.

$$\Delta^{(1)}(\mathbf{k},\mathbf{r}) \sim f_0(\mathbf{r})(k_x^2+k_y^2-2k_z^2), \quad H^{(1)} \sim \frac{T_{A1}-T}{\lambda_1}, \quad \lambda_1 = K_1 + K_{23}/6,$$

$$\Delta^{(2)}(\mathbf{k},\mathbf{r}) \sim f_2(\mathbf{r})(k_x-ik_y)k_z + f_0(\mathbf{r})(k_x+ik_y)k_z, \quad H^{(2)} \sim \frac{T_{E1}-T}{\lambda_2},$$

$$\lambda_2 = 3(K_1+K_{23}/4) - \sqrt{K_{23}^2/2 + (2K_1+K_{23}/2-K_{23}/4)^2}, \qquad (12)$$

where $f_n(\mathbf{r})$ is the wave function of the $n$th Landau level. Corresponding to the superconducting seeds $\Delta^{(1)}$ and $\Delta^{(2)}$ are different quantum numbers $N$ ($N=n+m$; Ref. 11) and different parities under reflection in the $x$–$y$ plane. Solutions (12) are thus not mixed in any order of the expansion of the energy in gradients. In the absence of an external pressure, with $T_{A1} > T_{E1}$, the lines $H^{(1)}(T)$ and $H^{(2)}(T)$ intersect at $\lambda_1 > \lambda_2$ (Fig. 2a). This condition holds in weak-coupling theory ($\lambda_1 = 1.67K_1$, $\lambda_2 = 1.1K_1$) and should continue to hold in the face of small deviations from that theory.

Let us consider the case $\mathbf{H} \perp \hat{z}$ now. By virtue of the uniaxial anisotropy of the original energy functional, $H_{c2}$ is isotropic in the basal plane of the crystal.Under the condition $\mathbf{H} \parallel \hat{x}$ the gradient terms are

$$F_{\rm grad}=K_1|\nabla_y\eta_x|^2+\left(K_1+\frac{1}{2}K_{23}\right)|\nabla_z\eta_x|^2+\left(K_1+\frac{1}{2}K_{23}\right)|\nabla_i\eta_y|^2$$
$$+\left(K_1+\frac{1}{6}K_{23}\right)|\nabla_y a_0|^2+\left(K_1+\frac{2}{3}K_{23}\right)|\nabla_z a_0|^2$$
$$-\frac{1}{2\sqrt{3}}[\eta_y^*((2K_2-K_3)\nabla_y\nabla_z+(2K_3-K_2)\nabla_z\nabla_y)a_0+\text{c.c.}], \qquad (13)$$

where $a_{\pm 1}=(\eta_x\pm i\eta_y)/\sqrt{2}$. Corresponding to the upper critical field are the following solutions, which differ in parity under reflection in the plane perpendicular to the magnetic field:

$$\Delta^{(3)}(\mathbf{k},\mathbf{r})\sim a_0(\mathbf{r})(k_x^2+k_y^2-2k_z^2)+\eta_y(\mathbf{r})k_yk_z, \quad H^{(3)}\sim\frac{T_{A1}-T}{\lambda_3(T)},$$

$$\Delta^{(4)}(\mathbf{k},\mathbf{r})\sim\eta_x(\mathbf{r})k_xk_z, \quad H^{(4)}\sim\frac{T_{\Xi 1}-T}{\lambda_4}. \qquad (14)$$

We can find $\lambda_4$ exactly: $\lambda_4 = \sqrt{K_1(K_1+K_{23}/2)}$. The slope of the $H^{(3)}(T)$ curve depends on the temperature, and near $T_c^+$, when we can ignore the admixture of the $k_yk_z$ component, we have $\lambda_3 = \sqrt{(K_1+K_{23}/6)(K_1+2K_{23}/3)} > \lambda_4$. A numerical calculation shows that the $H^{(3)}(T)$ dependence is slightly nonlinear in the Ginzburg–Landau regime. There should thus be a kink again in the case $\mathbf{H}\perp\mathbf{z}$. Comparing the equations above with experimental data,[11] we find the following relations between parameters: $K_2=K_3=2.2K_1$.

We have previously examined the need for additional lines of transitions in the $H$–$T$ plane going into the point of the kink on $H_{c2}(T)$ as well as possible types of symmetry breaking during transitions in vortex lattices.[11] At pressures $P>P^*$ the kink on $H_{c2}(T)$ disappears at the same time that the splitting of the superconducting transition disappears. The structure of the $H$–$T$ diagram is similar to that of the phase diagram for isotropic $d$-wave pairing (Fig. 2b).

It was mentioned in Ref. 13 that the angular dependence of the lower branch of $H_{c2}$ (i.e., the branch below the kink) is far stronger than the anisotropy of the upper branch. This fact can be explained in a natural way in our model: The anisotropy of $H_{c2}$ in weak fields is due to the splitting of $T_c$ and is described by Eqs. (12) and (14), while in strong fields the slight effect of the $T_c$ splitting in isotropic functional (1) is evidently unimportant, and $H_{c2}$ depends only weakly on direction. The assumption that crystal-field effects are small and the assumption of a nearly isotropic nontrivial pairing also explain the observed isotropy of $H_{c2}$ in another heavy-fermion superconductor: $UBe_{13}$, which has a cubic lattice. (If crystal-field effects are strong, then $H_{c2}$ should be strongly anisotropic in a cubic nontrivial superconductor.[14])

Indirect support for this model also comes from the tendency of the resistance (and thus of the effective-mass tensor of the conduction electrons) toward isotropy when pressure is applied.[15]

Some features of the $UPt_3$ phase diagram, such as the splitting of $T_c$ and the kink on $H_{c2}(T)$, can be explained by assuming an "accidental" degeneracy of the transition temperatures of two irreducible represents of the $D_{6h}$ group (an example with $A_{1g}$ and $E_{1g}$ was studied in Ref. 14). However, in order to explain the vertical line of transitions between the $\Delta_2(\mathbf{k})$ and $\Delta_3(\mathbf{k})$ phases in this case we would need a rigorously defined (and thus one more "accidental") relationship between the coefficients describing the interaction of order parameters. The model proposed above is thus preferable from that standpoint also.

This work was supported financially in part by the BMFT Foundation (Bonn; grant 13 #5750) and the American Physical Society through the International Science Foundation. One of us (I.L.) wishes to thank M. Sigrist for a useful discussion of this study.

[1] R. A. Fisher, S. Kim, B. F. Woodfield *et al.*, Phys. Rev. Lett. **62**, 1411 (1989).
[2] D. W. Hess, T. Tokuyasu, and J. A. Sauls, J. Phys. Cond. Matt. **1**, 8135 (1989).
[3] K. Machida, M. Ozaki, and T. Ohmi, J. Phys. Soc. Jpn. **58**, 4116 (1989).
[4] R. Joynt, V. P. Mineev, G. E. Volovik, and M. E. Zhitomirsky, Phys. Rev. **B42**, 2014 (1990).
[5] L. Taillefer, J. Flouquet, and G. G. Lonzarich, Physica **B169**, 257 (1991).
[6] B. G. Demcszyk, M. C. Aronson, B. R. Coles, and J. L. Smith, Philos. Mag. Lett. **67**, 85 (1993).
[7] P. A. Midgley, S. M. Hayden, L. Taillefer *et al.*, Phys. Rev. Lett. **70**, 678 (1993).
[8] A. Zangwill and R. Bruinsma, Comments Cond. Matt. Phys. **13**, 1 (1987).
[9] K. Scharnberg and R. A. Klemm, Phys. Rev. Lett. **54**, 2445 (1985).
[10] N. D. Mermin, Phys. Rev. **A9**, 868 (1974).
[11] M. E. Zhitomirskiĭ and I. A. Luk'yanchuk, Zh. Eksp. Teor. Fiz. **101**, 1954 (1992) [Sov. Phys. JETP **74**, 1046 (1992)]; I. A. Luk'yanchuk and M. E. Zhitomirsky, Physica **C206**, 373 (1993).
[12] N. H. van Dijk, A. de Visser, J. J. M. Franse *et al.*, *Proceedings of the International Conference on Strongly Correlated Systems* (Sendai, 1992).
[13] G. Bruls, D. Weber, B. Wolf *et al.*, Phys. Rev. Lett. **65**, 2294 (1990).
[14] L. I. Burlachkov, Zh. Eksp. Teor. Fiz. **89**, 1384 (1985) [Sov. Phys. JETP **62**, 800 (1985)].
[15] L. Taillerfer, J. Flouquet, Yu. P. Gaydukov, and N. P. Danilova, J. Magn. Magn. Mater. **108**, 138 (1992).

Translated by D. Parsons