# Effect of incommensurate modulations of the crystal structure on superconductivity

V. P. Mineev
*L. D. Landau Institute of Theoretical Physics, 142432 Chernogolovka, Moscow Oblast, Russia*
*Centre d'Etudes Nucleaires de Grenoble DRFMS/SPSMS, 85X-38041 Grenoble Cedex 24, France*

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The changes in the macroscopic symmetry of a crystal caused by a structural modulation, which is incommensurate with the lattice constants of the original crystal lattice, are analyzed. In particular, a study is made of the changes in the symmetry of superconducting phases with a multicomponent order parameter in the heavy-fermion superconductor $UPt_3$.

The reason for the splitting of the superconducting phase transition in $UPt_3$ is one of the main puzzles in the physics of heavy-fermion metals.[1] In a recent attempt to solve this puzzle by electron microscopy of $UPt_3$,[2] a modulation of the crystal lattice incommensurate with the lattice constants of this compound was observed. It was found that well-annealed samples, in which the superconducting transition is split, consist of uniform domains with an incommensurate structure $\sim 10^4$ Å in size. In $UPt_3$ single crystals which have not been annealed, on the other hand, in which a splitting of the transition is not observed, these domains are only slightly larger than the superconducting coherence length $\xi_0 \approx 120$ Å. Since unannealed crystals exhibit a smoothed jump in the specific heat as well as an unsplit transition, these observations probably signify a sort of nonuniform blurring of the superconducting transition in some temperature interval as the result of a decrease in the size of domains with a certain structural modulation, rather than an effect of an incommensurate modulation on the magnitude of the splitting of the superconducting transition.

The lack of direct experimental evidence for an effect of the incommensurate structure on the splitting of the superconducting transition in $UPt_3$ does not, of course, resolve the general question of possible changes in the superconducting state as the result of the appearance of incommensurate crystalline modulations. We know[3] that incommensurate modulations of crystal structure can alter the macroscopic symmetry of a crystal. The symmetry of superconducting phases with a nontrivial pairing, on the other hand, is determined primarily by the macroscopic symmetry of the directions in the crystal.[4] A change in this symmetry due to the appearance of structural modulations is equivalent to the application of an external field which disrupts the symmetry of the superconducting state. In the present letter we consider some examples of symmetry changes of this sort in the crystal class $D_{6h}$, to which $UPt_3$ belongs, and the effect of these changes on the superconductivity. Changes of this sort, which arise in hexagonal symmetry in an incommensurate phase of quartz, have been listed briefly in a review article.[5]

  

We assume that the density function $\rho(\mathbf{r})$ in a crystal deviates from the density of the unperturbed crystal, $\rho_0(\mathbf{r})$, which represents a set of plane waves:

$$\eta(\mathbf{r})=\rho(\mathbf{r})-\rho_0(\mathbf{r})=\sum_{I=1}^{N} f_i(\mathbf{q}_i\mathbf{r}+\psi_i). \tag{1}$$

Here $f_i(x)$ are periodic functions, which for simplicity we assume are sinusoids: $f_i(x)=\eta_i\cos x$. According to Midgley *et al.*,[2] the structural modulations in $UPt_3$ consist of three sets of waves: waves of type $A$, with wave vectors $\mathbf{q}_1$, $\mathbf{q}_2$, $\mathbf{q}_3$ satisfying $\mathbf{q}_1+\mathbf{q}_2+\mathbf{q}_3=0$, of type $B$ with wave vectors $\mathbf{q}_4$, $\mathbf{q}_5$, $\mathbf{q}_6$ satisfying $\mathbf{q}_4+\mathbf{q}_5+\mathbf{q}_6=0$; and of type $C$, with a wave vector $\mathbf{q}_7$. There are thus seven waves, which differ in directions, lengths, and amplitudes. The vectors $\mathbf{q}_i$ do not lie in the $(x,y)$ plane, which is orthogonal to the hexagonal $z$ axis, so a modulation $\eta(\mathbf{r})$ locally creates triclinic distortions of the hexagonal lattice. It turns out that these triclinic distortions are retained in the macroscopic symmetry of the directions of a hexagonal crystal with a structural modulation of the type described above.

To see the point argued above, we need to examine the interaction of density modulations with deformations of a crystal. We will retain only orthorhombic deformations, which are important for applications to superconductivity. For this purpose we substitute (1) into the invariant

$$(u_{xx}-u_{yy})\left[\left(\frac{\partial\eta}{\partial x}\right)^2-\left(\frac{\partial\eta}{\partial y}\right)^2\right]+4u_{xy}\frac{\partial\eta}{\partial x}\frac{\partial\eta}{\partial y}, \tag{2}$$

where $u_{ik}$ are components of the strain tensor. Taking an average over a volume with a linear dimension large in comparison with the periods of the spatial modulation, $2\pi/q_i$, we find

$$\sum_{i=1}^{n} q_i^2\eta_i^2\,[(\cos^2(\hat{q}_i\hat{x})-\cos^2(\hat{q}_i\hat{y}))(u_{xx}-u_{yy})+4\cos(\hat{q}_i\hat{x})\sin(\hat{q}_i\hat{y})u_{xy}]. \tag{3}$$

Minimizing the sum of this expression and of the elastic-strain energy, which is quadratic in the strain tensor $u_{ik}$, we find coordinate-independent equilibrium values of the components $(u_{xx}-u_{yy})$ and $u_{xy}$, which appear in the presence of structural-modulation waves. If the vectors $\mathbf{q}_i$ do not lie in the $(x,y)$ plane, we must of course supplement (2) with all other invariant combinations which are bilinear in $u_{ik}$ and $(\partial\eta/\partial r_i)$ $(\partial\eta/\partial r_k)$ . We then have the equilibrium values of the other components $u_{ik}$.

The quantities $u_{xx}-u_{yy}$ and $u_{xy}$ specify the orthorhombic strain tensor

$$\epsilon_{ik}=\begin{pmatrix} u_{xx} & u_{xy} \\ u_{xy} & -u_{yy}\end{pmatrix}. \tag{4}$$

When present in a hexagonal crystal, orthorhombic deformations split the superconducting transition into a state corresponding to either of the two 2D representations $E_1$ and $E_2$ of the hexagonal symmetry group.[6,7] In this case the Ginzburg–Landau functional describing the superconducting transition is

$$F=\alpha_0(T-T_{c0})|\vec{\psi}|^2+\beta_1|\vec{\psi}|^4+\beta_2|\vec{\psi}\,\vec{\psi}|^2+b\epsilon_k(\psi_i\psi_k^*+\text{c.c.}). \tag{5}$$

Under the conditions $\beta_2>0$ and $b>0$, there is first a transition to the $\psi\sim(0,1)$ phase at $T_{c1}=T_{c0}+(bu_{yy}/\alpha_0)$; then, at a lower temperature $T_{c2}<T_{c1}$, there is a transition to the $\psi\sim[ia(T-T_{c2}/T_{c2}),1]$ phase.

Another type of change in the macroscopic symmetry can be found from the interaction of density modulations and the polarization[1)] of the crystal along the $\hat{z}$ axis, $P_z$:

$$P_z\eta\left(\frac{\partial^3\eta}{\partial y^3}-3\frac{\partial^3\eta}{\partial y\partial x^2}\right)\left(\frac{\partial^3\eta}{\partial x^3}-3\frac{\partial^3\eta}{\partial x\partial y^2}\right). \tag{6}$$

Substituting (1) into (6) and taking an average, we find the contribution from the three waves of type $A$:

$$P_z\eta_1\eta_2\eta_3\cos(\psi_1+\psi_2+\psi_3)[q_2^3q_3^3\sin^3\theta_2\sin^3\theta_3\sin 3\varphi_2\sin 3\varphi_3+(1\leftrightarrow 2)+(3\leftrightarrow 1)], \tag{7}$$

where $\theta_i$ and $\varphi_i$ are respectively the polar and azimuthal angles of the vector $\mathbf{q}_i$. The contribution from the three waves of type $B$ is similar in form.

The interaction of the structural modulation with the polarization $P_z$, which is linear in $P_z$, disrupts the spatial parity; it gives rise to a special direction in the crystal, namely, the $z$ axis. As a result, a Lifshitz invariant appears in the Ginzburg–Landau functional for the two-component superconducting phase:

$$\psi_1\frac{\partial\psi_2^*}{\partial z}-\psi_2^*\frac{\partial\psi_1}{\partial z}+\text{c.c.} \tag{8}$$

This invariant must of course be considered jointly with the ordinary second-order gradient terms:

$$F=\alpha_0(T-T_{c0})|\vec{\psi}|^2+\beta_1|\vec{\psi}|^4+\beta_2|\vec{\psi}\,\vec{\psi}|^2+c\left(\psi_1\frac{\partial\psi_2^*}{\partial z}-\psi_2^*\frac{\partial\psi_1}{\partial z}+\text{c.c.}\right)+K\frac{\partial\vec{\psi}}{\partial z}\frac{\partial\vec{\psi}^*}{\partial z}. \tag{9}$$

Functional (9) is written without consideration of the orthorhombic distortions in (5). Such a functional describes a phase transition to a superconducting cholesteric phase

$$\vec{\psi}=\psi_0e^{i\varphi-i\theta(z)}(\mathbf{1},i),\quad \beta_2>0, \tag{10}$$

$$\vec{\psi}=\psi_0e^{i\varphi}\cos\theta(z)\sin\theta(z),\quad \beta_2<0. \tag{11}$$

Here $\theta(z)=\kappa z$, $\kappa=-c/K$, and $T_c=T_{c0}+(2c^2/\alpha_0K)$. In the case $\beta_2<0$, terms of sixth order, $\delta(|\psi_1|^6|-15|\psi_1|^4|\psi_2|^2+15|\psi_1|^2|\psi_2|^4-|\psi_2|^6)$, fix the phase of the cholesteric helix at low temperatures: $\theta(z)=\pi/6$ if $\delta>0$ and $\theta=0$ if $\delta<0$.

We wish to repeat that the appearance of incommensurate structural modulations in a crystal of hexagonal symmetry unavoidably creates orthorhombic distortions and disrupts the spatial parity of the crystal. Although these effects may be extremely small in magnitude, the orthorhombic distortions in a superconductor with a multicomponent order parameter (such as $UPt_3$) should cause a splitting of the phase transition to the superconducting state. The absence of an inversion center should lead to the appearance of superconducting cholesteric (helicoidal) phases.

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[1)]In the case of quartz, in which the spatial modulation itself has threefold symmetry around the $\hat{z}$ axis, it is sufficient to consider an interaction $P_z\eta^2[(\partial^3\eta/\partial y^3) - 3(\partial^3\eta/\partial y\partial x^2)]$.

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