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Strain distortion in anisotropic superconductors

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We point out that a uniform lattice strain is associated with the superconducting transition when the order parameter is anisotropic. The observation of such a strain would be a decisive signature of an anisotropic phase and may allow different phases to be distinguished. We show, in a simple model, that the effect may be expected to be large in heavy-fermion materials with small shear moduli.

The discovery of superconductivity in heavy-fermion systems[1] has touched off a debate over the nature of the order parameter in these materials. Some workers have proposed that the pairing is of the conventional s-wave type,[2] arguing that the electron-phonon coupling is large. Others favor p-wave pairing,[3-5] pointing to the evidence that spin fluctuations dominate the excitation spectrum at low energies.[4,5] One then has a number of possibilities. Two possibilities which have been put forward are an Anderson-Brinkman-Morel (ABM) phase,[5] as in the A phase of condensed ^{3}He, and a polar phase.[6] These come from the analogy to ^{3}He, but these possibilities are strongly modified when spin-orbit coupling and crystal symmetry are taken into account.[7-10]

Experimental identification of these phases is greatly hindered by the fact that the order parameter does not directly couple to external probes. Thus, one must rely on indirect consequences of the ordering, such as measurements of the specific heat, NMR, and transport properties. Certain theoretical assumptions must be made to calculate these properties, even when given the form of the order parameter. Unfortunately, however, we do not yet have a good understanding of the quasiparticles of the normal system, and therefore of strong-coupling effects, disorder, etc., and their influence on the low-temperature properties.[11] This makes progress in the identification of phases difficult.

The purpose of this paper is to point out that the measurement of a uniform lattice strain can provide proof of the existence of an anisotropic phase, and also give qualitative information about the wave-vector dependence of the gap function.

The reasoning is as follows. The energy of condensation is given at $T=0$ K by

$$E_c = -\tfrac{1}{4}\sum_{\mathbf{k}} \delta(\epsilon_{\mathbf{k}}-\mu)\,\mathrm{Tr}[\Delta^\dagger(\mathbf{k})\Delta(\mathbf{k})]\,. \tag{1}$$

Here $\epsilon_{\mathbf{k}}$ is the quasiparticle energy, $\mathbf{k}$ is the wave vector, μ is the chemical potential, and we allow the 2×2 order parameter Δ to have nontrivial $\mathbf{k}$ dependence. It is evident from this expression that the system will prefer to maximize its density of states in directions where the gap is large. It can do this by expanding in these directions. Thus, for a polar state, where Δ vanishes in the equatorial plane and has maxima at the poles, we expect a tetragonal phase with $c/a>1$. The ABM state, whose gap has converse properties, will favor a c/a ratio of less than one. Such general considerations determine the strain distortion for any gap function.

To do explicit calculations, we will adopt a single-band tight-binding model. Thus, our chief assumption is that the heavy Fermi liquid may be described by an effective band as in some recent theories.[2,12] This allows us to bury our ignorance of the nature of the quasiparticles in a single parameter $\chi \equiv \partial \ln T/\partial \ln a$, where T is the transfer matrix element and a is the lattice constant. We treat a simple cubic lattice (appropriate for UBe_{13}) with an unperturbed Fermi surface which is spherical. (The analysis would not be significantly different for a Fermi surface of more general cubic symmetry.) In this model, we may replace $\epsilon_{\mathbf{k}}$ in Eq. (1) by $k^2/2m^* + \sum_i (\chi/2m^*)(\Delta a_i/a)k_i^2$. Δa_i is the change of the lattice constant in the ith direction on relaxing to the ground state. μ also depends on the volume, but this turns out to be a smaller effect.

If we now ignore the dependence of Δ on length changes (we will discuss this hypothesis below), then it is straightforward to compute the dependence of the condensation energy on the volume change $\Delta V/V=(1/a)\sum_i \Delta a_i$ and the strain distortions $\gamma_x \equiv 1/a\,(a_x - \frac{1}{2}a_y - \frac{1}{2}a_z)$, γ_y, and γ_z. The results for the two most easily visualized cases are

$$E_c(\mathrm{ABM}) = E_0 + \chi E_0\left(\frac{-4\Delta V}{3V} + \frac{\gamma_z}{3}\right)\,,$$

for an ABM gap which has $\mathbf{k}$ dependence $\mathrm{Tr}(\Delta^\dagger\Delta)\sim(k_x^2+k_y^2)$, and

$$E_c(\mathrm{polar}) = E_0 + \chi E_0\left(\frac{-4\Delta V}{3V} - \frac{2\gamma_z}{3}\right)$$

for a polar gap with $\mathrm{Tr}(\Delta^\dagger\Delta)\sim k_z^2$. E_0 is the condensation energy in the absence of strain. $E_0<0$ and $\chi = \partial \ln T/\partial \ln a < 0$. Hence, in the ground state, $\gamma_z(\mathrm{ABM})<0$ and $\gamma_z(\mathrm{polar})>0$, as expected.

To obtain estimates of the magnitude of these changes we need to include the elastic contribution, which for a cubic crystal is

$$E_{\mathrm{el}} = \tfrac{1}{6}(c_{11}+2c_{12})\left(\frac{\Delta V}{V}\right)^2 + (c_{11}-c_{12})(\gamma_x^2+\gamma_y^2+\gamma_z^2)\,,$$

if we limit ourselves to diagonal distortions. c_{11} and c_{12} are the usual elastic constants. Minimization of the total energy then leads to

$$\frac{\Delta V}{V} = \frac{4\chi E_0}{(c_{11}+2c_{12})}\,,\quad \gamma_z = \frac{-\chi E_0}{6(c_{11}-c_{12})}\quad (\mathrm{ABM}),$$

and

$$\frac{\Delta V}{V} = \frac{4\chi E_0}{(c_{11}+2c_{12})}\,,\quad \gamma_z = \frac{\chi E_0}{3(c_{11}-c_{12})}\quad (\mathrm{polar})\,.$$

The order of magnitude of these quantities in UBe_{13} can be estimated from $E_0 \sim -N(0)\Delta^2 \sim -T_c C_n(T_c) \sim -10^5$ erg/cm^3, where $N(0)$ is the density of states at the Fermi surface and C_n is the normal-state specific heat. χ is estimated to be about -40 from other measurements.[3,13,14] The elastic constants are taken from pure Be: $c_{11}+2c_{12}=3.6\times10^{12}$ dyn/cm^2 and $c_{11}-c_{22}=2.7\times10^{12}$ dyn/cm^2. So $\Delta V/V \sim 10^{-6}$, about an order of magnitude larger than the $\Delta V/V$ associated with superconductivity in a conventional system. This is to be expected because of the very high density of states and correspondingly large energy of condensation. This is in accord with thermal expansion measurements on polycrystalline samples.[15] The corresponding value of the tetragonal distortion parameter, $|\gamma_z| \sim 10^{-7}$, implies an anisotropy of about 10%.

As noted above, in the presence of strong spin-orbit coupling, the crystal symmetry will determine the possible forms of the order parameter. In Table I, we tabulate the results for strain distortions for the states given by Ueda and Rice.[9] The results for volume changes are the same as for the polar and ABM states given above. As can be seen, the presence or absence of a strain anomaly, and its sign, give one considerable information about the nature of the superconductivity. In fact, Table I does not exhaust the information one can obtain. In our model, electronic energies depend only on nearest-neighbor bond lengths. In actuality, they depend also on bond angles, and these degrees of freedom will also couple to the order parameter, allowing more general strains than purely orthorhombic. For example, the cases

$$\mathbf{d}=\frac{1}{\sqrt{6}}[\hat{\mathbf{x}}(k_y-k_z)+\hat{\mathbf{y}}(k_z-k_x)+\hat{\mathbf{z}}(k_x-k_y)]$$

and the two involving c_1,c_2,c_3 have gap zeros in the [111] direction. Thus, one expects rhombohedral phases for these. The coupling is likely to be rather smaller for these cases, however. In general, any lowering of the cubic symmetry indicates an anisotropic superconducting order parameter. Blount[10] has tabulated the point group for which the order parameter forms a one-dimensional representation, for each possible phase. The $T=0$ K crystal structure must fall into the class determined by this group. Since the deviations from cubic may be too small to be detected by x-ray measurements, however, this is probably not of much practical importance.

In all these calculations, we have assumed that the only effect of a change in lattice constants is to alter the density of states. In general, however, one expects the coupling constant to be changed as well, which will also contribute to the condensation energy. Since we have little microscopic understanding of the quasiparticle interactions at present, this contribution is impossible to calculate. However, it seems reasonable to suppose that it will depend only on the *volume* and not on the volume-preserving distortions. Thus, we regard our results for volume changes to be only order-of-magnitude estimates. The results for the γ_i, on the other hand, are much more firm.

TABLE I. Strain distortions for p-wave states in a simple cubic crystal, given in units of $\chi E_0/(c_{11}-c_{12})$. The gap is specified according to the convention $\Delta(k_x,k_y,k_z)=i\mathbf{d}\cdot\boldsymbol{\sigma}\sigma_y$, where the σ_i are the Pauli matrices. $(c_1,c_2,c_3)=(1/\sqrt{2}+i/\sqrt{6},-1/\sqrt{2}+i/\sqrt{6},-2i/\sqrt{3})$.

d	Orthorhombic strains
$\frac{1}{\sqrt{3}}(\hat{\mathbf{x}}k_x+\hat{\mathbf{y}}k_y+\hat{\mathbf{z}}k_z)$	None
$\frac{1}{\sqrt{2}}(\hat{\mathbf{x}}k_x-\hat{\mathbf{y}}k_y)$	$-\frac{1}{6}=\gamma_z$
$\frac{1}{\sqrt{6}}(2\hat{\mathbf{z}}k_z-\hat{\mathbf{x}}k_x-\hat{\mathbf{y}}k_y)$	$\frac{1}{6}=\gamma_z$
$\frac{1}{\sqrt{3}}(\hat{\mathbf{z}}k_z+e^{-2\pi i/3}\hat{\mathbf{x}}k_x+e^{2\pi i/3}\hat{\mathbf{y}}k_y)$	None
$\frac{1}{\sqrt{2}}(\hat{\mathbf{y}}k_z-\hat{\mathbf{z}}k_y)$	$-\frac{1}{6}=\gamma_x$
$\frac{1}{\sqrt{6}}[\hat{\mathbf{x}}(k_y-k_z)+\hat{\mathbf{y}}(k_z-k_x)+\hat{\mathbf{z}}(k_x-k_y)]$	None
$\frac{1}{2}[\hat{\mathbf{x}}(c_2k_z-c_3k_y)+\hat{\mathbf{y}}(c_3k_x-c_1k_z)+\hat{\mathbf{z}}(c_1k_y-c_2k_x)]$	None
$\frac{1}{2}[\hat{\mathbf{x}}(k_y+ik_z)-(\hat{\mathbf{y}}-i\hat{\mathbf{z}})k_x]$	$\frac{1}{12}=\gamma_x$
$\frac{1}{\sqrt{2}}(\hat{\mathbf{y}}k_z+\hat{\mathbf{z}}k_y)$	$-\frac{1}{6}=\gamma_x$
$\frac{1}{\sqrt{6}}[\hat{\mathbf{x}}(k_y+k_z)+\hat{\mathbf{y}}(k_z+k_x)+\hat{\mathbf{z}}(k_x+k_y)]$	None
$\frac{1}{2}[\hat{\mathbf{x}}(c_2k_z+c_3k_y)+\hat{\mathbf{y}}(c_3k_x+c_1k_z)+\hat{\mathbf{z}}(c_1k_y+c_2k_x)]$	None
$\frac{1}{2}[\hat{\mathbf{x}}(k_y-ik_z)+(\hat{\mathbf{y}}-i\hat{\mathbf{z}})k_x]$	$\frac{1}{12}=\gamma_x$

The calculations have been carried out at zero temperature, but may be easily extended by noting that the effects are proportional to $\mathrm{Tr}(\Delta^\dagger\Delta)$, and so, near the critical temperature, to T_c-T. To go to finite magnetic field, we recall that the systems of interest are type-II superconductors. In the mixed state there will be a reduction due to the normal fraction. We also note that field cooling will be necessary to align the domains of an anisotropic superconductor if macroscopic strains are to be observed. Another method of alignment might be the application of uniaxial stress.

We conclude that the observation of anisotropic strain would give direct evidence for p-wave pairing in the heavy-fermion superconductors. The sign of the effect can also help to distinguish between different p-wave states. The effects are larger than volume changes in conventional superconductors, and should be observable.

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