In-plane upper critical field anisotropy in Sr$_2$RuO$_4$ and CeIrIn$_5$

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Experiments on tetragonal Sr$_2$RuO$_4$ and CeIrIn$_5$ indicate the presence of superconductivity with a multi-component superconducting order parameter. Such an order parameter should exhibit an in-plane anisotropy in the upper critical field near the superconducting transition temperature that does not occur for single-component superconductors. Here, this anisotropy is determined from microscopic calculations for arbitrary gap functions. It is shown that this anisotropy is generally not small and, in some cases, independent of impurity scattering. Furthermore, this anisotropy is calculated for many detailed microscopic models of Sr$_2$RuO$_4$. For these models this anisotropy is found to be large, which is in sharp contrast to the small anisotropy observed experimentally. However, an accidental cancellation of the anisotropy for gaps on different Fermi surface sheets can lead to a result that is consistent with experiment.

One of the central issues in the field of unconventional superconductivity is the identification of the order parameter symmetry. This issue can usually only be addressed by determinations of the phase of the order parameter (such as through Josephson junction experiments). However, in the case that the Cooper pair wave functions have more than one complex degree of freedom, other experimental signatures can reveal the pairing symmetry. In this paper one of these signatures, the upper critical field anisotropy for fields in the basal plane, is explored for tetragonal superconductors. This anisotropy was established by Gor’kov on phenomenological grounds. Such an anisotropy, for which $dH_{c2}/dT_{c}$ is not equal for the magnetic field applied along the (0, 0) and the (1, 1, 0) directions, cannot occur for superconducting order parameters that have only one complex degree of freedom (for example conventional s-wave superconductors or $d_{x^2−y^2}$-wave superconductors). Consequently, this provides a clear test of the pairing symmetry. For tetragonal materials, there exist two possible pairing states that exhibit this property. One is the spin triplet $E_u$ representation which can be described a gap function of the form (note that this is not the most general form) $\Delta(k) = \tilde{\eta}[\eta f_x(k) + \eta_2 f_y(k)]$, where in the simplest case (for a cylindrical Fermi surface) $f_x(k) = k_x$ and $f_y(k) = k_y$. Such a gap function is believed to describe the pairing state in Sr$_2$RuO$_4$ (see below). The other pairing state is the spin-singlet $E_g$ representation which can be described by a gap function of the form $\Psi(k) = \eta f_x(k) + \eta_2 f_y(k)$, where $f_{xz}(k) = k_x k_z$ and $f_{yz}(k) = k_y k_z$ in the simplest case. In this article, the anisotropy is determined within microscopic theories with arbitrary gap functions. It is shown that this anisotropy is generally not small and consequently easily observable. Furthermore, it is shown that for the $E_u$ representation and for some theories for the $E_u$ representation, this anisotropy is impurity independent. Application of these results to Sr$_2$RuO$_4$ and CeIrIn$_5$ are discussed and detailed calculations for Sr$_2$RuO$_4$ are also presented. Prior to discussing the anisotropy, an overview of the superconductivity in Sr$_2$RuO$_4$ and CeIrIn$_5$ is given.

The oxide Sr$_2$RuO$_4$ has a structure similar to high $T_c$ materials and was observed to be superconducting by Maeno et al. in 1994. It has been established that this superconductor is not a conventional s-wave superconductor: NQR measurements show no indication of a Hebel-Slichter peak value of 1.5 K by non-magnetic impurities of Luke et al. (see below). This has prompted a recent series of proposals that the gap function has the form $\Delta(k) = \tilde{\eta}[\eta f_x(k) + \eta_2 f_y(k)]$, where $f_x(k_0) = f_y(k_0) = 0$ for a set of points $k_0$ that form a line on the Fermi surface, or are very anisotropic. These gap functions are all formally of the same $E_u$ symmetry. The fact that these theories all have the same symmetry implies that there exist experimental signatures that will be common to all of them. In particular, the upper critical field anisotropy discussed above should exist. Recently, such an anisotropy has been observed by Mao et al. It was determined that $1 − H_{c2}^{(100)} / H_{c2}^{(110)} = 0.03$ at a temperature of 0.35$K (≈ T_c / 5)$, $1 − H_{c2}^{(100)} / H_{c2}^{(110)}$ was observed to
change sign as $T \to T_c$, and appears to remain small for $T$ near $T_c$. In this paper, the anisotropy near $T_c$ will be calculated for a variety of models.

Very recently, it has been reported that μSR experiments of Heffner et. al. have revealed spontaneous fields in the Meissner state of tetragonal CeIrIn$_5$. Just as in the case for Sr$_2$RuO$_4$ above, this indicates that the superconducting gap function is either of $E_u$ symmetry or of $E_g$ symmetry. Consequently, both pairing symmetries are considered in this article.

The free energy for the $E_u$ and $E_g$ representations of $D_{4h}$ is given by

$$f = -\alpha|\vec{\eta}|^2 + \beta_1|\vec{\eta}|^4/2 + \beta_2(\eta_1\eta_2 - \eta_2\eta_1)^2/2$$

$$+ \beta_3|\eta_1|^2|\eta_2|^2 + \kappa_1|D_x\eta_1|^2 + |D_y\eta_2|^2$$

$$+ \kappa_2(|D_y\eta_1|^2 + |D_z\eta_2|^2)$$

$$+ \kappa_3(|D_x\eta_1|(D_y\eta_2)^* + h.c.)$$

$$+ \kappa_4(|D_y\eta_1|(D_z\eta_2)^* + h.c.) + \frac{h^2}{2(8\pi)}.$$  

where $D_j = \nabla_j - \frac{2ie}{\hbar c} A_j$, $\hbar = \nabla \times A$, and $A$ is the vector potential. The stable homogeneous solutions are easily determined. There are three phases: (a) $\vec{\eta} = (1,i)/\sqrt{2}$ ($\beta_2 > 0$ and $\beta_2 > \beta_3/2$), (b) $\vec{\eta} = (1,0)$ ($\beta_3 > 0$ and $\beta_2 < \beta_3/2$), and (c) $\vec{\eta} = (1,1)/\sqrt{2}$ ($\beta_3 < 0$ and $\beta_2 < 0$). The weak-coupling approximation predicts that phase (a) is stable since this phase minimizes the number of nodes in the order parameter [note that in exceptional circumstances, phase (a) may be degenerate with phase (b) and (c) in the weak-coupling limit, for example in the theory of Ref. 30].

For an external magnetic field applied in the basal plane, the upper critical field can be determined and is found to be

$$H_{c2}(\theta) = \frac{\alpha hc}{e\sqrt{2\kappa_5}} \sqrt{\kappa_2 + \kappa_1 - \sqrt{(\kappa_1 - \kappa_2)^2 \cos^2(2\theta) + (\kappa_3 + \kappa_4)^2 \sin^2(2\theta)}}$$

where $\theta$ is the angle between the magnetic field and the crystallographic $a$ axis. From the above expression, the ratio of $H_{c2}$ for the field along the $(1,0,0)$ direction to that for the field along the $(1,0,0)$ direction is given by

$$\frac{H_{c2}^{(1,1,0)}}{H_{c2}^{(1,0,0)}} = \sqrt{(\kappa_1 + \kappa_2 - |\kappa_3 + \kappa_4|)/2\min(\kappa_2, \kappa_1)}$$

where $\min(\kappa_2, \kappa_1)$ means the minimum of $\kappa_2$ and $\kappa_1$. Note that Sigrist has also determined an additional anisotropy that occurs due to spin-orbit coupling. This additional anisotropy introduces a correction to Eq. 3 that vanishes as $T \to T_c$, so it is not considered here.

Here, this anisotropy is determined in the weak-coupling approximation. This approximation is reasonable for Sr$_2$RuO$_4$ since $T_c/T_F \approx 10^{-4}$, however it is not clear whether or not this approximation is valid for CeIrIn$_5$. Using a gap function of the form $d(\mathbf{k}) = \sqrt{2} \eta_1 f_x(\mathbf{k}) + \eta_2 f_y(\mathbf{k})$ for the $E_u$ representation and introducing isotropic impurity scattering within a $T$-matrix approximation yields (the details will be given in a later publication)

$$\kappa_1 = \frac{\pi N(0)}{2} \sum_{n \geq 0} \frac{1}{(\omega_n + 1)^2} \left[ \langle f_x^2 v_x^2 \rangle + \frac{1}{\omega_n} \langle f_x v_x v_y \rangle \right]$$

$$\kappa_2 = \frac{\pi N(0)}{2} \sum_{n \geq 0} \frac{1}{(\omega_n + 1)^2} \langle f_y^2 v_y^2 \rangle$$

$$\kappa_3 = \frac{\pi N(0)}{2} \sum_{n \geq 0} \frac{1}{(\omega_n + 1)^2} \times$$

$$\langle f_x f_y v_x v_y \rangle + \frac{1}{\omega_n} \langle f_x v_x v_y \rangle$$

$$\kappa_4 = \frac{\pi N(0)}{2} \sum_{n \geq 0} \frac{1}{(\omega_n + 1)^2} \langle f_x f_y v_x v_y \rangle$$

$$\kappa_5 = \frac{\pi N(0)}{2} \sum_{n \geq 0} \frac{1}{(\omega_n + 1)^2} \langle f_y^2 v_y^2 \rangle$$

where $\omega_n = (2n + 1)\pi T$, $N(0)$ is the density of states at the Fermi surface, $\Gamma = 1/\tau_N$ is half of the scattering rate, $v_i$ are the components of the Fermi velocity, and the brackets $\langle \rangle$ denote an average over the Fermi surface. It has also been assumed that $\langle f_x^2 + f_y^2 \rangle = 1$. The terms proportional to $\Gamma$ in $\kappa_1$ and $\kappa_3$ are vertex corrections (which have the same form as those that arise in the calculation of current-current correlation functions). In the clean limit, this gives

$$\frac{H_{c2}^{(1,1,0)}}{H_{c2}^{(1,0,0)}} = \sqrt{\frac{\langle f_x^2 v_x^2 \rangle + \langle f_y^2 v_y^2 \rangle - 2\langle f_x f_y v_x v_y \rangle}{2\min(\langle f_x^2 v_x^2 \rangle, \langle f_y^2 v_y^2 \rangle)}}.$$  

(3)
For $\kappa_2 < \kappa_1$ and $\kappa_3 + \kappa_4 > 0$, this ratio is independent of the impurity concentration. The requirement that $\kappa_2 < \kappa_1$ implies for the field along $(1,0,0)$ that $(\eta_1, \eta_2) = \eta(r)(1,0)$ [for $\kappa_2 > \kappa_1$ $(\eta_1, \eta_2) = \eta(r)(0,1)$] while the requirement that $\kappa_3 + \kappa_4 > 0$ implies that for the field along the $(1,1,0)$ direction that $(\eta_1, \eta_2) = \eta(r)(1,1)$ [if $\kappa_3 + \kappa_4 < 0$ then $(\eta_1, \eta_2) = \eta(r)(1,-1)$]. Note that as the magnetic field is decreased, there will exist a second order phase transition due to a change in the order parameter structure. For example, for the field along $(1,0,0)$ and for $\kappa_3 < \kappa_1$ there will be a second order transition with decreasing field where the component $(\eta_1, \eta_2) \propto (0,1) \neq 0$. Such a transition reduces the number of nodes in the gap structure which is why it occurs.

For the $E_g$ representation using $\Psi(k) = (\eta_1 f_{xz} + \eta_2 f_{yz})$ gives

$$
\kappa_1 = \frac{\pi N(0)}{2} \sum_{n \geq 0} (f_{xz}^2 v_x^2) \\
\kappa_2 = \frac{\pi N(0)}{2} \sum_{n \geq 0} \frac{1}{(\omega_n + 1)^2} (f_{yz}^2 v_y^2) \\
\kappa_3 = \frac{\pi N(0)}{2} \sum_{n \geq 0} \frac{1}{(\omega_n + 1)^2} \times \\
(\langle f_{xz} f_{yz} v_x v_y \rangle) \\
\kappa_4 = \frac{\pi N(0)}{2} \sum_{n \geq 0} \frac{1}{(\omega_n + 1)^2} (f_{xz} f_{yz} v_x v_y) \\
\kappa_5 = \frac{\pi N(0)}{2} \sum_{n \geq 0} \frac{1}{(\omega_n + 1)^2} (f_{xz}^2 v_x^2)
$$

The main difference with the $E_u$ representation is that no vertex corrections appear. For an arbitrary impurity concentration this gives

$$
\frac{H_{c2}^{(1,1,0)}}{H_{c2}^{(1,0,0)}} = \sqrt{\frac{(f_{xz}^2 v_x^2) + (f_{yz}^2 v_y^2)}{2 \min((f_{xz}^2 v_x^2), (f_{xz}^2 v_y^2))}}.
$$

This ratio is independent of the impurity concentration. These results (and the more detailed calculations below) indicate that the anisotropy is not generally small and should therefore be easily detected. It would be of interest to look for this anisotropy in CeIrIn$_3$.

It is informative to determine the anisotropy for existing microscopic theories in the clean limit. Since no such theories for CeIrIn$_3$ exist to date, the remainder of the analysis concentrates on Sr$_2$RuO$_4$. To do this the electronic dispersion must be given as input for the form of the gap function. Initially, consider theories that for simplicity use a cylindrical Fermi surface. For a gap function with nodes in the basal plane $(f_x, f_y) = [(k_x^2 - k_y^2)k_x, -(k_x^2 - k_y^2)k_y]$ the $H_{c2}^{(1,1,0)}/H_{c2}^{(1,0,0)} = 0.58$. For an anisotropic but fully gapped gap function: $(f_x, f_y) = [\sin(k_x), \sin(k_y)]$ with $k_F = 0.9\pi\frac{\sqrt{2}}{2}$. $H_{c2}^{(1,1,0)}/H_{c2}^{(1,0,0)} = 0.53$. These estimates indicate that the anisotropy should be easily observable if the gap contains nodes in the basal plane or is anisotropic (these possibilities might be expected due to recent experiments that indicate nodes in the gap). This in contrast to the experimental results of Mao et al.

A more careful investigation below indicates that the anisotropy can accidentally be hidden, even for theories with nodes in the plane.

To consider more realistic models, a tight binding approach is used to describe the electronic dispersion near the Fermi surface. Local-density approximation band-structure calculations reveal that the density of states near the Fermi surface is due mainly to the four Ru $4d$ electrons in the $t_{2g}$ orbitals. There is a strong hybridization of these orbitals with the O $2p$ orbitals giving rise to antibonding $\pi^*$ bands. The resulting bands have three quasi-2D Fermi surface sheets labelled $\alpha$, $\beta$ and $\gamma$ (see Fig. 1). To model these Fermi surface sheets, the following tight-binding dispersions are used:

$$
\epsilon_\gamma = \epsilon_\gamma^0 - 2t_x (\cos k_x + \cos k_y) - 4t_{xy} \cos k_x \cos k_y \\
\epsilon_{\alpha,\beta} = \epsilon_{\alpha,\beta}^0 - t_{\alpha,\beta} (\cos k_x + \cos k_y) \pm \sqrt{\epsilon_{\alpha,\beta}^0 (\cos k_x - \cos k_y)^2 + 16t_{\alpha,\beta}^2 \sin^2 k_x \sin^2 k_y}
$$

In following tight binding values are used: $(\epsilon_\gamma^0, t_{\gamma,\gamma}, \tilde{t}_\gamma) = (-0.4, 0.4, 0.12)$ for the $\gamma$ sheet and the values $(\epsilon_{\alpha,\beta}^0, t_{\alpha,\beta,\alpha}, \tilde{t}_{\alpha,\beta}) = (-0.3, 0.25, 0.0375)$ for the $\{\alpha, \beta\}$ sheets. Table 1 shows the anisotropy ratio for gap functions found in various theories for Sr$_2$RuO$_4$.

Note that for the $\alpha$ and $\beta$ bands the gap functions with $v_x$ replaced by $\sin k_x$ were not included (as they were for the $\gamma$ band). This is due to quasi one-dimensional nature of the $\alpha$ and $\beta$ sheets. In particular, $v_{x,\alpha} \propto \sin k_x [1 + \sgn(\cos k_x - \cos k_y)]/2 \neq \sin k_x$ in the one-dimensional limit. It is $v_x$, not $\sin k_x$, which would be the gap function for a one-dimensional nearest neighbor pair interaction. This is supported by the calculations of Kuroki et al. where the $(f_x, f_y) = (v_x, v_y)$ basis functions on the $\alpha$ sheet of Ref. gives a good approximation to the crib-shaped...
can appear simultaneously in the pairing state of Sr$_2$RuO$_4$ and E. The surface sheet must be larger than that on the Fermi surface, and may be present in CeIrIn$_5$. Also it is shown that for E$_g$ gap functions and for some E$_a$ gap functions, this anisotropy is independent of impurity scattering. For Sr$_2$RuO$_4$, it is shown that an accidental cancellation of this anisotropy can occur if the γ sheet of the Fermi surface is largely responsible for the superconductivity.

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FIG. 1. Fermi surface of Sr$_2$RuO$_4$ using the tight binding parameters in this paper ($k_x$ and $k_y$ are in units $\pi/a$ where $a$ is the lattice spacing). Moving out from the $k = (0,0)$ point, first the $\beta$ sheet, then the $\gamma$ sheet, and finally the $\alpha$ sheet are crossed.

| $f_x(k)$ | $f_y(k)$ | Fermi Surface | $\frac{H_{c2}^{100}}{H_{c2}^{110}}$ | Impurity Dependent |
|----------|----------|---------------|----------------------------------|--------------------|
| $v_x$    | $v_y$    | $\gamma$     | 0.50                            | no                 |
| $(\cos k_x - \cos k_y)v_x$ | $-(\cos k_x - \cos k_y)v_y$ | $\gamma$     | 0.86                            | yes                |
| $\sin k_x \sin k_y v_y$ | $\sin k_x \sin k_y v_x$ | $\gamma$     | 0.31                            | yes                |
| $\sin k_x$ | $\sin k_y$ | $\gamma$     | 0.36                            | yes                |
| $(\cos k_x - \cos k_y) \sin k_x$ | $(\cos k_x - \cos k_y) \sin k_y$ | $\gamma$     | 0.51                            | yes                |
| $\sin^2 k_y \sin k_x$ | $\sin^2 k_x \sin k_y$ | $\gamma$     | 0.24                            | no                 |
| $v_x$    | $v_y$    | $\alpha$     | 2.0                             | no                 |
| $(\cos k_x - \cos k_y)v_x$ | $-(\cos k_x - \cos k_y)v_y$ | $\alpha$     | 3.9                             | yes                |
| $\sin k_x \sin k_y v_y$ | $\sin k_x \sin k_y v_x$ | $\alpha$     | 1.2                             | yes                |
| $v_x$    | $v_y$    | $\beta$      | 2.5                             | no                 |
| $(\cos k_x - \cos k_y)v_x$ | $-(\cos k_x - \cos k_y)v_y$ | $\beta$      | 5.23                            | yes                |
| $\sin k_x \sin k_y v_y$ | $\sin k_x \sin k_y v_x$ | $\beta$      | 1.52                            | yes                |

TABLE I. Upper critical field anisotropy for various gap functions for Sr$_2$RuO$_4$. Note that the normalization of the gap functions has not been included here. The column called Impurity Dependent states whether or not $H_{c2}^{100}/H_{c2}^{110}$ depends upon impurity scattering.