Nontrivial interplay of superconductivity and spin-orbit coupling in noncentrosymmetric ferromagnets

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(Received 29 August 2008; revised manuscript received 24 September 2008; published 5 November 2008)

Motivated by the recent discoveries of ferromagnetic and noncentrosymmetric superconductors, we present a mean-field theory for a superconductor that *both* lacks inversion symmetry and displays ferromagnetism, a scenario which is believed to be realized in UIr. We study the interplay between the order parameters to clarify how superconductivity is affected by the presence of ferromagnetism and spin-orbit coupling. One of our key findings is that the spin-orbit coupling seems to enhance both ferromagnetism and superconductivity in all spin channels. We discuss our results in the context of the heavy fermion superconductor UIr and analyze possible symmetries of the order parameter by the group theory method.

DOI: 10.1103/PhysRevB.78.172502 PACS number(s): 74.20.Rp, 74.20.Mn, 74.50.+r, 74.70.Tx

In the past decade, a number of superconductors have been discovered that are called "unconventional" as they fall outside the Bardeen-Cooper-Schrieffer (BCS) paradigm of electron-phonon mediated pairing with an isotropic gap. Of those, UPt_3 (Ref. 1) and Sr_2RuO_4 (Ref. 2) were the compounds to have been confirmed as triplet p-wave superconductors. More recently, a ferromagnetic (FM) superconductor was discovered in UGe_2 under pressure,[3] where the presence of an internal FM moment strongly suggests that only the equal-spin triplet pairing survives. In this latter example both the time-reversal and the gauge symmetry due to SC order are spontaneously broken, which made UGe_2, as well as its cousins URhGe (Ref. 4) and UCoGe (Ref. 5) an exciting avenue for theoretical and experimental research.

For spin-triplet pairing, Anderson noticed[6] that inversion symmetry is required to obtain a pair of degenerate states $c_{\mathbf{k}}^{\dagger}|0\rangle$ and $c_{-\mathbf{k}}^{\dagger}|0\rangle$ capable of forming a Cooper pair. It was therefore surprising that superconductivity was discovered in the heavy fermion compound $CePt_3Si$ which lacks inversion symmetry.[7] It soon became clear, however, that in the case of a noncentrosymmetric crystal, the spin-orbit coupling (SOC) mixes different spin states, so that the division into triplet and singlet symmetry of the SC order parameter becomes meaningless. A bulk of theoretical work exists that has provided a symmetry-based phenomenology to explain this in details.[8–12] The symmetry of the superconducting (SC) gap in this and other unconventional superconductors is presently a matter of intense investigation.[13–16]

An intriguing question is what happens if time-reversal symmetry is broken in a crystal that lacks a center of inversion. Can such a material become a superconductor? This question was answered affirmatively when superconductivity was discovered in the noncentrosymmetric ferromagnetic compound UIr under pressure.[17] The symmetry of the SC order parameter and its connection to FM nevertheless remains unclear, which motivates the present study. Spontaneous symmetry breaking in condensed-matter systems is conceptually of immense importance, as it may provide clues for what could be expected in systems belonging to vastly different areas of physics. The study of a condensed-matter system such as UIr with multiple broken symmetries is likely to have impact on a number of disciplines of physics, including such disparate phenomena as mass differences between elementary particles and extremely dilute ultracold atomic gases.

In this Brief Report, we study a model system of a noncentrosymmetric superconductor with substantial spin-orbit coupling, which at the same time exhibits itinerant ferromagnetism. The origin of the SOC may be either that the crystal structure lacks a center of inversion, such as in UIr, or due to a thin-film geometry where the breakdown of inversion symmetry near the surface induces transverse electrical fields, leading to the well-known Rashba SOC.[18] Our model should therefore be relevant both to the noncentrosymmetric and centrosymmetric heavy fermion compounds, since the SOC is considerable in any case due to the high atomic number. Specifically, materials that exhibit coexistence of SC and FM order and where SOC is large include UGe_2,[3] URhGe,[4] UCoGe,[5] and UIr.[17] For this model, we construct a mean-field theory, solve the saddle-point equations for the order parameters, and study the effect of spin-orbit coupling on the superconducting order parameters. Finally, we discuss application of this model to the case of UIr.

To label the SOC+FM split bands, it is possible to introduce a *pseudospin* basis in which the normal-state Hamiltonian is diagonalized. In the original spin basis, the SC matrix order parameter is characterized, in analogy to the p-wave state,[19] by a vector $\mathbf{d_k}$ and a scalar $\mathbf{\Delta_s}$ so that $\Delta_{\alpha\beta}(\mathbf{k})=i\Delta_s\sigma_y+[(i\mathbf{d_k}\cdot\boldsymbol{\sigma})\sigma_y]_{\alpha\beta}$. Note that, unlike the usual p-wave SC, a singlet component of the gap will also be present since antisymmetric SOC in general mixes the parity of the order parameter.

We now proceed to write down the effective Hamiltonian $\hat{H}=\hat{H}_N+\hat{H}_{SC}$ for our system. In the normal state, the Hamiltonian in momentum-space reads[20]

$$\hat{H}_N=H_0+\sum_{\mathbf{k}\alpha\beta}[c_{\mathbf{k}\alpha}^{\dagger}(\varepsilon_{\mathbf{k}}\hat{1}-h\hat{\sigma}_z+\hat{\boldsymbol{\sigma}}\cdot\mathbf{g_k})_{\alpha\beta}c_{\mathbf{k}\beta}], \qquad (1)$$

where $H_0=INM^2/2$. Above, the dispersion relation $\varepsilon_{\mathbf{k}}$ is measured from chemical potential μ, and the magnetization $M=|\mathbf{M}|$ is taken along the easy axis, while $h=IM$ is the exchange splitting of the bands and $\mathbf{g_k}$ is the SOC vector. When superconductivity coexists with FM, the SC pairing is generally believed to be nonunitary,[21] characterized by $\mathbf{d_k}\times\mathbf{d_k^*}\neq 0$. In such a scenario, the SC order parameter couples to the spontaneous magnetization $\mathbf{M}$ through a term $\gamma\mathbf{M}\cdot\mathbf{d_k}\times\mathbf{d_k^*}$ in the free energy, where the sign of γ is determined by the gradient of the DOS at Fermi level[22] and $\langle\mathbf{S_k}\rangle=i\mathbf{d_k}\times\mathbf{d_k^*}$ is the spin associated with the Cooper pair. Thus, for $\gamma<0$ it is expected that a SC pairing state obeying $i\mathbf{d_k}\times\mathbf{d_k^*}\parallel\mathbf{M}$ is energetically favored, implying that $\mathbf{d_k}$ must be complex valued. Our model captures broken time-reversal symmetry in addition to antisymmetric SOC. As shown by Anderson,[6] the presence of the latter is detrimental to spin-triplet SC pairing state, unless $\mathbf{d_k}\parallel\mathbf{g_k}$. In our case, it is obvious that a nonunitary SC pairing state cannot satisfy this condition since $\mathbf{d_k}$ is complex, whereas $\mathbf{g_k}$ must be real for the Hamiltonian to be Hermitian.

The SOC vector reads $\mathbf{g_k}=-\mathbf{g_{-k}}$, and we introduce $g_\mathbf{k}=\mathbf{g}_{\mathbf{k},x}-i\mathbf{g}_{\mathbf{k},y}$ for later use. We consider the SOC in the Rashba form, namely $\mathbf{g_k}=\lambda(k_y,-k_x,0)$. This corresponds to a situation where an asymmetric potential gradient is present along the $\hat{\mathbf{z}}$ axis, and is also the scenario realized in noncentrosymmetric $CePt_3Si$.[11] We have introduced fermion operators $\{\hat{c}_{\mathbf{k}\sigma}\}$ in a basis $\hat{\varphi}_\mathbf{k}=[c_{\mathbf{k}\uparrow},c_{\mathbf{k}\downarrow}]^T$.

Diagonalizing the normal-state Hamiltonian yields the quasiparticle excitations $\tilde{E}_{\mathbf{k}\sigma}=\varepsilon_\mathbf{k}-\sigma\sqrt{h^2+\lambda^2k^2}$, which due to the SOC are characterized by the pseudospin $\sigma=\pm1$. For later use, we define $\mathcal{N}_\mathbf{k}=[1+\lambda^2k^2/(h+\sqrt{h^2+\lambda^2k^2})^2]^{-1/2}$. The superconducting pairing is now assumed to occur between the excitations described by $\hat{\tilde{\varphi}}_\mathbf{k}$. Due to the presence of antisymmetric spin-orbit coupling, this automatically leads to a mixed-parity SC state in the original spin basis. To see this, we introduce

$$\hat{H}_{\text{SC}}=\frac{1}{2N}\sum_{\mathbf{kk}'\sigma}V_{\mathbf{kk}'\sigma}\tilde{c}^\dagger_{\mathbf{k}\sigma}\tilde{c}^\dagger_{-\mathbf{k}\sigma}\tilde{c}_{-\mathbf{k}'\sigma}\tilde{c}_{\mathbf{k}'\sigma},\tag{2}$$

and perform a standard mean-field decoupling, which after an additional diagonalization yields the total Hamiltonian in the superconducting state: $\hat{H}=H_0+\Sigma_{\mathbf{k}\sigma}(\tilde{E}_{\mathbf{k}\sigma}-E_{\mathbf{k}\sigma}-\tilde{\Delta}_{\mathbf{k}\sigma}\tilde{b}^\dagger_{\mathbf{k}\sigma}+2\eta^\dagger_{\mathbf{k}\sigma}\eta_{\mathbf{k}\sigma})/2$, where $E_{\mathbf{k}\sigma}=(\tilde{E}^2_{\mathbf{k}\sigma}+|\tilde{\Delta}_{\mathbf{k}\sigma}|^2)^{1/2}$ and $\{\eta^\dagger_{\mathbf{k}\sigma},\eta_{\mathbf{k}\sigma}\}$ are fermion operators in the new basis. The merit of this procedure is that we can now obtain simple self-consistency equations for the gaps $\tilde{\Delta}_{\mathbf{k}\sigma}$, which may then be transformed back to the gaps in the original spin-basis $\hat{\varphi}_\mathbf{k}$ by means of the unitary transformation $P_\mathbf{k}$. We assume a chiral p-wave symmetry for the gaps with a corresponding pairing potential $V_{\mathbf{kk}'\sigma}=-g_{\text{sc}}e^{i\sigma(\phi-\phi')}$, where $\tan\phi=k_x/k_y$. The motivation for this is that this choice ensures that the condition $\mathbf{d_k}\parallel\mathbf{g_k}$ is satisfied exactly for $h\to0$, and corresponds to a fully gapped Fermi surface which favors the condensation energy. The gaps obtain the form $\tilde{\Delta}_{\mathbf{k}\sigma}=-\sigma\tilde{\Delta}_{\sigma,0}e^{i\sigma\phi}$ and we find a self-consistency equation of the standard BCS form with a cutoff ω on the pairing-fluctuation spectrum which we do not specify further. Moreover, $N^\sigma(\varepsilon)$ is the pseudospin-resolved density of states (DOS) for the $\tilde{E}_{\mathbf{k}\sigma}$ ($\sigma=\pm$) bands of the quasiparticle excitations.[23] Introducing the total DOS at the Fermi level for a normal metal $N_0=mV\sqrt{2m\mu}/\pi^2$ and defining
$c=g_{\text{sc}}N_0/2$, the analytical solution for the gaps reads $\tilde{\Delta}_{\sigma,0}=2\omega\exp\{-1/[cR_\sigma(0)]\}$, $R_\sigma(\varepsilon)=2N^\sigma(\varepsilon)/N_0$. With the analytical solution for $\tilde{\Delta}_{\sigma,0}$ in hand, we may exploit the unitary transformation $P_\mathbf{k}$ to express the superconducting gaps in the original spin basis as follows:

$$\Delta_{\mathbf{k}\uparrow}=-e^{i\phi}[\tilde{\Delta}_{\uparrow,0}(\mathcal{N}^\uparrow_\mathbf{k})^2+\tilde{\Delta}_{\downarrow,0}(\mathcal{N}^\downarrow_\mathbf{k})^2\lambda^2k^2_\downarrow(0)\Lambda^2_{\mathbf{k}\downarrow}],$$

$$\Delta_{\mathbf{k}\downarrow}=e^{-i\phi}[\tilde{\Delta}_{\downarrow,0}(\mathcal{N}^\downarrow_\mathbf{k})^2+\tilde{\Delta}_{\uparrow,0}(\mathcal{N}^\uparrow_\mathbf{k})^2\lambda^2k^2_\uparrow(0)\Lambda^2_{\mathbf{k}\uparrow}],$$

$$\Delta_{\mathbf{k}\uparrow\downarrow}=-\sum_\sigma\tilde{\Delta}_{\sigma,0}(\mathcal{N}^\sigma_\mathbf{k})^2\lambda|k_\sigma(0)|\Lambda_{\mathbf{k}\sigma},\quad\sigma=\pm1,\tag{3}$$

where we have defined $\mathcal{N}^\sigma_\mathbf{k}=\mathcal{N}_{\mathbf{k}=\mathbf{k}^\sigma(0)}$ and $\Lambda_{\mathbf{k}\sigma}=[h+\sqrt{h^2+\lambda^2k^2_\sigma(0)}]^{-1}$. Note that in the original spin basis, the superconducting order parameter is in general a mixture of triplet ($\Delta_{\mathbf{k}\sigma}$) and singlet ($\Delta_{\mathbf{k}\uparrow\downarrow}$) components. The self-consistency equation for the magnetization is

$$h+\frac{\tilde{I}}{4}\sum_\sigma\int\frac{\sigma d\varepsilon R^\sigma(\varepsilon)h\varepsilon}{\sqrt{[h^2+\lambda^2k^2_\sigma(\varepsilon)](\varepsilon^2+\tilde{\Delta}^2_{\sigma,0})}}=0,\tag{4}$$

where the integration is over the bandwidth and $\tilde{I}=IN_0$. Equations (3) and (4) are the main analytical results of this work.

Let us briefly investigate some important limiting cases of Eq. (3). In the absence of spin-orbit coupling ($\lambda\to0$), one finds $\mathcal{N}^\sigma_\mathbf{k}\to1$ and $\Delta_{\mathbf{k}\sigma}=\tilde{\Delta}_{\mathbf{k}\sigma}$ while $\Delta_{\mathbf{k}\uparrow\downarrow}=0$, such that we reproduce the results of Refs. 20 and 24. In the absence of an exchange energy ($h\to0$), one finds that $\mathcal{N}^\sigma_\mathbf{k}\to1/\sqrt{2}$ and $\Delta_{\mathbf{k}\uparrow}=-e^{i\phi}(\tilde{\Delta}_{\uparrow,0}+\tilde{\Delta}_{\downarrow,0})/2$, $\Delta_{\mathbf{k}\downarrow}=e^{-i\phi}(\tilde{\Delta}_{\uparrow,0}+\tilde{\Delta}_{\downarrow,0})/2$, and $\Delta_{\mathbf{k}\uparrow\downarrow}=(\tilde{\Delta}_{\downarrow,0}-\tilde{\Delta}_{\uparrow,0})/2$. As demanded by consistency, the triplet gaps are equal in magnitude since there is no exchange field and the singlet component is nonzero since $\tilde{\Delta}_{\uparrow,0}\neq\tilde{\Delta}_{\downarrow,0}$ in general. Finally, Eq. (4) reproduces the well-known Stoner criterion $\tilde{I}\geq1$ for the onset of FM in the absence of SOC and superconductivity ($\lambda\to0,g_{\text{sc}}\to0$).

We now focus on the general case in which $h\neq0$ and $\lambda\neq0$. First of all, we must specify the range of the parameters in the problem that corresponds to a physically realistic scenario. We allow h to range, in principle, from 0 to μ, the latter denoting a fully polarized ferromagnet. As a convenient measure of the strength of SOC, we introduce the dimensionless quantity $\alpha_{\text{soc}}\equiv\sqrt{2\lambda^2m/\mu}$ which has a direct physical interpretation; namely, it is the ratio of the SOC (at E_F) to the Fermi energy μ. The parameter α_{soc} is allowed to vary from 0 to δ, where δ denotes a fraction of the Fermi energy. We take $\delta=0.5$ as a sensible upper limit. Note that generically, the SOC strength at the Fermi level is different for the two quasiparticle bands, and moreover depends on h. For a given value of h, one may derive that $\lambda\leq\delta\mu/[2\mu m+\sqrt{2m^2(h^2+\delta^2\mu^2)}]^{1/2}$ ensures that the spin-orbit energy is less than $\delta\times\mu$ for both quasiparticle bands.

In Figs. 1(a)–1(d), we present the self-consistent solutions for the order parameters in Eqs. (3) and (4) as a function of

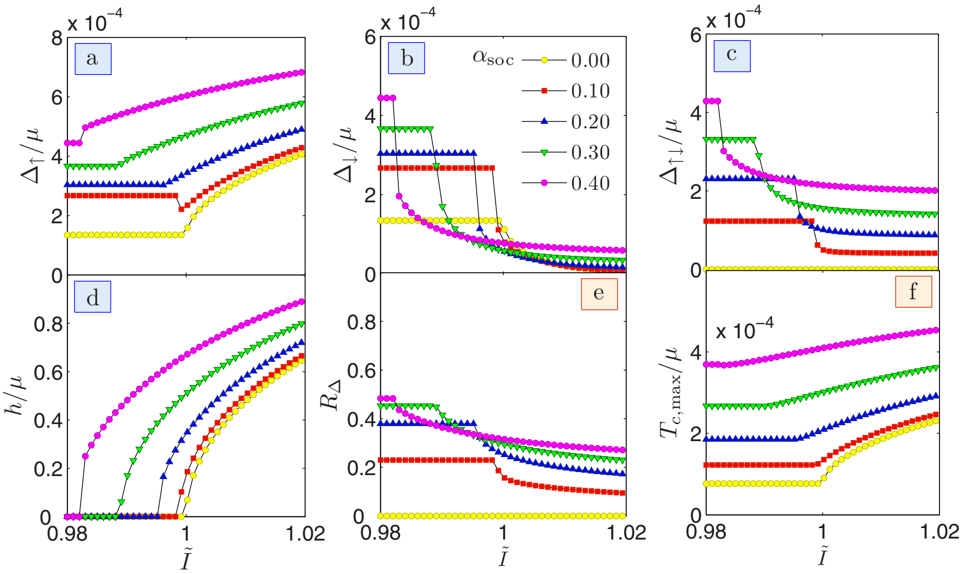

FIG. 1. (Color online) Self-consistent solution of the order parameters [(a)–(d)] as a function of the FM exchange parameter $\tilde{I}$, the ratio between the singlet and triplet gaps (e) $R_\Delta = \Delta_{\uparrow\downarrow}/(\Delta_\uparrow + \Delta_\downarrow)$, and the maximal critical temperature (f) $T_{c,\max}$ as a function of the FM exchange parameter $\tilde{I}$.

the FM exchange parameter $\tilde{I}$ for several values of $\alpha_{\rm soc}$. We have defined $\Delta_\sigma = |\Delta_{\mathbf{k}\sigma}|$ and $\Delta_{\uparrow\downarrow} = |\Delta_{\mathbf{k}\uparrow\downarrow}|$, and fixed $\omega/\mu = 0.01$ and $m/\mu = 5\times 10^4$ with $c=0.2$, which are standard choices. For $\alpha_{\rm soc}=0$, the onset of FM occurs at $\tilde{I}=1.0$ which lifts the degeneracy of $\Delta_\uparrow$ and $\Delta_\downarrow$, while $\Delta_{\uparrow\downarrow}$ is always zero. Upon increasing $\alpha_{\rm soc}$, it is interesting to note that the PM-FM transition occurs at lower values of $\tilde{I}$, indicating that spin-orbit coupling favors ferromagnetic ordering. For $\alpha_{\rm soc}\neq 0$, it is seen that $\Delta_{\uparrow\downarrow}$ is also nonzero, although it becomes suppressed at the onset of ferromagnetism. A common feature for all gaps is that they increase with $\alpha_{\rm soc}$ in the absence of ferromagnetism *and* deep inside the ferromagnetic phase $\tilde{I} \geq 1.02$. In the intermediate regime, there are crossovers between the gaps for different values of $\alpha_{\rm soc}$ due to the different onsets of ferromagnetic order. By comparing the behavior between the gaps for increasing $\tilde{I}$ with $\alpha_{\rm soc}\neq 0$, one infers that $\Delta_\downarrow$ and $\Delta_{\uparrow\downarrow}$ eventually saturate at a constant nonzero value, while $\Delta_\uparrow$ continues to increase steadily. This is quite different from the case when $\alpha_{\rm soc}=0$, where the minority spin-gap goes to zero rapidly with increasing $\tilde{I}$. This seems to suggest that the presence of spin-orbit coupling in the system ensures the survival of the minority-spin gap $\Delta_\downarrow$ and the singlet gap $\Delta_{\uparrow\downarrow}$ even though the FM exchange energy becomes strong.

In Figs. 1(e) and 1(f), we plot the ratio of the singlet and triplet gaps, defined as $R_\Delta = \Delta_{\uparrow\downarrow}/(\Delta_\uparrow + \Delta_\downarrow)$, and the maximal critical temperature $T_{c,\max}$ for the onset of superconductivity. It is seen from the left panel that R_Δ increases with $\alpha_{\rm soc}$ in the PM regime, suggesting that the singlet component becomes more prominent in the system as compared to the triplet gaps. However, at the onset of FM order, R_Δ decreases since the singlet component becomes suppressed by the Zeeman splitting. In the right panel, one observes that $T_{c,\max}$ increases both with $\alpha_{\rm soc}$ and $\tilde{I}$. Our findings suggest that the presence of antisymmetric SOC, originating from, e.g., noncentrosymmetricity of the crystal structure, *enhances both* the tendency toward ferromagnetism and the magnitude of the SC gaps in all spin channels. In the absence of spin-orbit coupling, it was shown in Ref. 20 that the simultaneous coexistence of FM and nonunitary triplet superconductivity is the thermodynamically favored state as compared to the pure normal, FM, or SC state. Since the presence of spin-orbit coupling is seen to enhance both the FM and SC order parameters, it is reasonable to expect that the coexistent state is still thermodynamically the most favorable one even when $\alpha_{\rm soc}\neq 0$.

Out of the known noncentrosymmetric superconductors, UIr is the only compound that is also a ferromagnet. This material, which is ferromagnetic at ambient pressure, develops superconductivity in a narrow pressure region around $P\sim 2.6$ GPa right next to the FM-PM quantum phase transition, with a maximum SC transition temperature $T_{\rm SC} \sim 0.14$ K.[17] At this pressure, the saturated magnetic moment was measured to be $0.07\mu_B$ per U atom, and such a small value clearly indicates the itinerant character of the ferromagnetism, presumably due to $5f$ electrons of uranium. UIr crystallizes in the monoclinic structure (space group $P2_1$) which lacks inversion symmetry, and the FM moment is Ising-like, oriented along the $[10\bar{1}]$ direction in the (ac) plane.

Given the proximity of the SC state in UIr to the PM transition, one may probably consider the magnetization h as a perturbation on top of the SOC-split bands. Neglecting the effect of the former, it is known[12] that even in the case of noncentrosymmetric superconductors (and $h=0$), the band energies still satisfy the relation $\varepsilon_\beta(\mathbf{k}) = \varepsilon_\beta(-\mathbf{k})$ due to the time-reversal symmetry of the single-electron Hamiltonian. As a consequence, the SC order parameter on the βth sheet of the Fermi surface transforms according to one of the irreducible representations of the normal state point group. In the case of UIr, the point group $\mathbf{C}_2$ has two one-dimensional irreducible representations, denoted A and B. Then the SC order parameter is an odd function $\Delta(-\mathbf{k}) = -\Delta(\mathbf{k})$ given by[25] $\Delta_\beta^{A,B}(\mathbf{k}) \propto t(\mathbf{k})\phi_\beta^{A,B}(\mathbf{k})$, where $t(\mathbf{k})$ is an odd phase factor[26] and the basis functions $\phi^{A,B}$ are even in $\mathbf{k}$. Denoting the rotation axis of the $\mathbf{C}_2$ group as z (this actually corresponds to b axis in case of UIr), the even functions ϕ_A and ϕ_B can then be cast in the following form: $\phi_A(\mathbf{k}) = (k_z^2 + C)u_1(\mathbf{k})$, and $\phi_B(\mathbf{k}) = k_z[k_x u_2(\mathbf{k}) + k_y u_3(\mathbf{k})]$, where C is some constant and $\{u_i(\mathbf{k})\}$ are arbitrary even functions of k_x, k_y, k_z. Function ϕ_A generically has no nodes, whereas ϕ_B has two point nodes at the poles ($k_x = k_y = 0$) and a line of nodes at the equator. The symmetry argument does not allow one to determine which pairing channel is realized, however, the experimental observation of the strong pair-breaking effect due to disorder[17] indicates that the gap must be anisotropic, possibly favoring the gap with the nodes such as $\Delta_B(\mathbf{k})$.

One way of experimentally probing the symmetry of the superconducting order parameter in UIr would be by means of transport properties such as Josephson tunneling or point-contact spectroscopy. In particular, it has recently been shown that the presence of multiple gaps in superconductors with broken inversion symmetry should manifest itself through clear signatures at bias voltages corresponding to the sum and difference of the singlet and triplet components.[20,27,28] We expect similar behavior in the present case, at least when the ferromagnetism is weak, and point-contact spectroscopy data could then be compared with the predictions for R_Δ in Fig. 1(e). Alternatively, it should be possible to directly probe the spin texture of the superconducting order parameter by studying the effect of an externally applied magnetic field when the paramagnetic limitation dominates, e.g., in a thin-film structure, where the orbital mechanism of destroying superconductivity is suppressed.[29]

In summary, we have developed a mean-field model for a superconductor lacking inversion symmetry and displaying itinerant ferromagnetism. Specifically, we have investigated the interplay between ferromagnetism and asymmetric spin-orbit coupling and how these affect superconducting order, which in general is a mixture of a singlet and triplet components. Our main results are the analytical expression Eqs. (3) and (4) and the belonging discussion. We find that spin-orbit coupling may *enhance* superconductivity in both the singlet and triplet channels in addition to favoring the Stoner criterion for the ferromagnetic instability. We have applied these considerations to the heavy fermion superconductor UIr, together with group-theoretical analysis of the symmetry of the SC order parameter.

The authors are grateful to M. Dzero for bringing Ref. 10 to our attention. A.H.N. was supported by the U.S. NSF Grant No. DMR 0605935. J.L. and A.S. were supported by the Norwegian Research Council Grants No. 158518/431 and No. 158547/431 (NANOMAT), and Grant No. 167498/V30 (STORFORSK).

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