The recently discovered heavy fermion superconductor CePt$_3$Si\cite{2,3,4,5,6,7,8,9,10} has triggered many experimental and theoretical studies\cite{10,11}. There are two features which have caused this attention: the absence of inversion symmetry; and the comparatively high upper critical magnetic field ($H_{c2}$). Broken inversion symmetry (parity) has a pronounced effect on the quasiparticle states through the splitting of the two spin degenerate bands. This influences the superconducting phase, which usually relies on the formation of pairs of electrons in degenerate quasiparticle states with opposite momentum. The availability of such quasiparticle states is usually guaranteed by the many body wavefunction of Cooper pairs of electrons in degenerate quasi-particle states with opposite momentum. The many body wavefunction with the helical order. We use the single particle Hamiltonian

$$H_0 = \sum_{k,s,s'} [\xi_k\sigma_0 + \alpha g_k \cdot \sigma + \mu_B H \cdot \sigma] c_{ks}^\dagger c_{ks'},$$

where $c_{ks}^\dagger$ creates (annihilates) an electron with momentum $k$ and spin $s$. The band energy $\xi_k = \epsilon_k - \mu$ is measured relative to the chemical potential $\mu$, $\alpha g_k \cdot \sigma$ introduces the antisymmetric spin-orbit coupling with $\alpha$ as a coupling constant (we set $\langle g_k^2 \rangle = 1$ where $\langle . \rangle$ is an average over the Fermi surface), and $\mu_B B \cdot \sigma$ gives the Zeeman coupling. The crucial term in $H_0$ is $\alpha g_k \cdot \sigma$, which is only permitted when inversion symmetry is broken ($g_k$ satisfies $g_k = -g_{-k}$ due to time reversal symmetry). This term destroys the usual two-fold spin degeneracy of the bands by splitting the band into two spin-dependent parts with energies $E_{k,\pm} = \xi_k \pm \alpha |g_k|$. The spinors are determined by the orientation of the corresponding $g_k$. The general pairing interaction is

$$H_{\text{pair}} = \frac{1}{2} \sum_{k,k',q,s_1,s_2} V(k,k') \xi_{k+q/2,s_1} \xi_{k-q/2,s_2} c_{k+q/2,s_1}^\dagger c_{-k-q/2,s_2}^\dagger c_{k'-q/2,s_1} c_{k'+q/2,s_2},$$

in the experimental data is surprising in this context.

In this letter we examine the mixed phase close to the upper critical field. Using the crystal symmetry of CePt$_3$Si, we show that the high-field superconducting phase has pronounced differences for field-directions parallel and perpendicular to the c-axis. For the field parallel to the c-axis, the paramagnetic limiting is basically absent and the vortex phase is quite conventional. While for the perpendicular field direction, the field can induce a phase which gives rise to an additional phase factor in the many body wavefunction $e^{i\mathbf{q}\cdot\mathbf{R}}$ with $\mathbf{q}$ perpendicular to the applied field: a helical vortex phase. We also propose a Josephson junction experiment that can be used to detect this helical order. In particular, we predict that Josephson current will exhibit a magnetic interference pattern for a magnetic field applied perpendicular to the junction normal. We also discuss unusual magnetic effects associated with the helical order.

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two-band solution has both a spin-triplet and a spin-singlet gap function when $\alpha \neq 0$ (this is a consequence of the broken parity symmetry). We will consider the limit $\alpha >> \mu B H$ and keep only terms up to order $\mu B H/\alpha$ (a good approximation for CePt$_3$Si). We restrict ourselves to choices of $V(k, k')$ that corresponds to spin-singlet pairing in the $\alpha = 0$ limit. This restriction allows us to use Eq. (5) even if $H \neq 0$, which considerably simplifies the notation.

With the two band pairing interaction of Eq. (5), the linearized gap equation becomes

$$\Delta_\alpha (k, q) = -T \sum_{n, k'} \sum_{\beta} V_{\alpha, \beta}(k, k') G^{0}_{\beta}(k') + q/2, i\omega_n) G^0_{\beta}(-k' + q/2, -i\omega_n) \Delta_\beta (k', q)$$

(4)

where $G^{0}_{\beta}(k, \omega_n) = [i\omega_n + \xi_k \pm \alpha |g_k|]^{-1}$. Setting $\Delta_+(k, q) = e^{i\phi_k} \Delta_+(k, q)$ and $\Delta_-(k, q) = -e^{-i\phi_k} \Delta_-(k, q)$ results in the simplified two-band equation with the interaction

$$V = V(k, k')(\sigma_0 - \sigma_x)/2.$$  

(5)

The factors $\hat{g}$ in Eq. (5) do not appear because of Pauli exclusion and the assumed singlet form of $V(k, k')$ in the $\alpha = 0$ limit. We denote the density of states on the two Fermi surfaces by $N_+ = N \cos^2(\delta/2)$ and $N_- = N \sin^2(\delta/2)$. We can write $\Delta_\alpha (k, q) = \psi_{\Gamma, \alpha}(q) f_{\Gamma}(k)$, where Eq. (5) implies that $\psi_{\Gamma, +}(q) + \psi_{\Gamma, -}(q) = 0$. With $\psi_{\Gamma, +}(q) = -\psi_{\Gamma, -}(q) = \psi(q)$ and the proper Fourier transform of the gap equation keeping gauge invariance, we find the following equation determining the upper critical field

$$\Psi(R) \ln t \frac{1}{t} = \int_0^\infty \frac{du}{\sinh(\nu u)} \langle |f_{\Gamma}(k)|^2 |\cos(\tilde{\mu} \bar{H} \cdot \tilde{g} u) + i \cos \delta \sin(\tilde{\mu} \bar{H} \cdot \tilde{g} u)| e^{-|\vec{\nu}_\perp|^2 \bar{H} u^2/2 \epsilon_v \Pi \Delta \sqrt{H} u e^{-\nu \Pi} \Delta \sqrt{H} u - 1} \rangle \Psi(R)$$

where $t = T/T_c$, $\bar{H} = H v_F^2/(2\pi T_c T^2)$, $\tilde{\mu} = \mu B T_c T^2 (v_2^2 - v_1^2)$, $v_+ = (v_1^2 + iv_2^2)$, $v_\perp = (v_1 + iv_2)/\sqrt{2}$, $v_1, 2$ are components of the Fermi velocity perpendicular to the magnetic field, $\Pi \Delta = (D_1 + i D_2) H/\sqrt{2}$, $\Pi \Delta = \Phi_0/(2\pi H)$, and $D_1 = -i \partial_b - 2e A_1/c$. The upper critical field $H_{c2}$ is found by expanding $\Psi(R) = \sum_n a_n \phi_n(R)$ ($\phi_n(R)$ are the usual Landau levels).

In the following we take a spherical Fermi surface. For CePt$_3$Si this will not be the case, but the overall geometry of the Fermi surface does not qualitatively change our results. We also take $g_k = \sqrt{3}/2(-k_y, k_x, 0)$ as the lowest order term in $k$ allowed by symmetry and consider the case $V(k, k') = V_0$ for isotropic $s$-wave pairing. Our results will hold for any pairing symmetry as the Ginzburg Landau (GL) theory discussed later will demonstrate.

For the field along the $c$-axis, $g \cdot H = 0$ so $H_{c2}$ is independent of the Zeeman field and there is no paramagnetic effect (note that in principle there can be a paramagnetic effect since there are $g_z$ allowed by symmetry that contain a $g_z$ component, however such terms are expected to be small). The solution of the upper critical field problem is identical to that carried out by Helfand and Werthamer and is plotted in Fig. 1. However, for fields perpendicular to the $c$-axis unusual properties occur, which can be best illustrated by a GL theory with free energy density

$$f = -a |\psi|^2 + \frac{\beta}{2} |\psi|^4 + \frac{1}{2m} D \psi^2 + \frac{1}{2m_e} D_2 \psi^2 + e n \cdot B \times [\psi (D \psi)^* + \psi^*(D \psi)] + \frac{B^2}{8\pi}$$

(6)

where $a = a_0(T_c - T)$, $D = (D_x, D_y)$, $n$ is the unit vector oriented along the $c$-axis, and $B = \nabla \times A$. Eq. (5) applies
to all possible pairing symmetries with a single complex order parameter, as discussed also by Samokhin. The lack of inversion symmetry allows for the existence of the term proportional to $\epsilon$ (for a discussion of other related terms see Ref. 15). This term induces a spatially modulated solution in a uniform magnetic field. The GL equation for the order parameter $\tilde{\Psi}(R) = e^{iq \cdot R} \Psi(R)$ in a field is identical to the zero-$\epsilon$ GL equation with $\Psi(R)$, where
\[
q = -2m\epsilon n \times B
\] (a microscopic expressions for $q$ is given below). Consequently, the upper critical field solution in the GL limit is $\Psi(R) = \phi_0(R)e^{iq \cdot R}$. We call this phase the helical vortex phase. The helical order coincides with an increase in the upper critical field ($B = H$):
\[
T_c(H) = T_c - \frac{\pi H}{\phi_0 \sqrt{mn} a_0} + \frac{m e^2(n \times H)^2}{2a_0}.
\] The expression for the supercurrent density is
\[
J = e\nabla \times [B - 4\pi m]/4\pi = J_0 + 4\epsilon e(n \times B)|\Psi|^2
\] where $J_0$ is the usual supercurrent density in the GL limit and $m = \frac{\mu_0}{4\pi} n \times J_0$ is the magnetization due to the $\epsilon$ term Eq. 6. The usual boundary condition on the order parameter is given by $J = 0$ through the boundary. The appearance of $m$ in Eq. 9 is highly unusual in GL theory and has some consequences that are discussed later. Note that if $|\Psi|$ and $B$ are spatially uniform then $J = 0$ for $q$ given by Eq. 4 the helical phase carries no current. The possibility of this helical order has been raised in the context of thin film or interface superconductivity where the vector potential can be neglected. As discussed below, we find here that it can play a very important role in the vortex phase.

The increase in $H_{c2}$ due to the appearance of the helical plays an important role in the microscopic theory. Since
\[
q \cdot H = 0,
\] we can expand $\phi_0(R)e^{iq \cdot R} = \sum_n b_n(q)\phi_n(R)$ where $b_n = (iql_H)^n e^{-(ql_H)^2/4\sqrt{2}mn}$. Our numerical microscopic solution has this form and near $T_c$ we find
\[
q = 2\mu_B H \cos \delta \frac{\langle \hat{q}(k) \cdot \hat{x} \rangle_{F,V}}{(k^2_{F,V})^{1/2}},
\] for $f_{V}(k) = 1$ this gives $ql_H = 0.373\alpha_M \cos \delta \sqrt{H/H_{c2}^0}$ where $\alpha_M = \sqrt{H_{c2}^0}/H_P$ is the Maki parameter, $H_{c2}^0$ is the upper critical field for $\mu_B = 0$ (this coincides with the $H_{c2}$ for the field along the $c$-axis), and $H_P = \Delta/(\mu_B \sqrt{2})$. For $f_{V}(k) = k_z^2 - k_y^2$, Eq. 10 gives $ql_H = 0.418\alpha_M \cos \delta \sqrt{H/H_{c2}^0}$. The enhancement of $H_{c2}$ due to the helical order can be substantial as Fig. 1 shows. Our numerical results show $ql_H$ can be larger than one, which implies that the helical wavelength becomes less than the spacing between vortices. Fig. 1 is for $\alpha_M = 3$ which is slightly smaller than $\alpha_M = 3.8$ that follows from the measurements of Ref. 8. The helical order changes with varying $\cos \delta$. For $\cos \delta = 0$ the density of states are the same on both Fermi surfaces and no helical order appears (labelled ‘in-plane (no helical)’ in Fig.1); while for $\cos \delta = 1$, $ql_H$ is maximum (this corresponds to the curve labelled ‘in-plane (helical)’ in Fig. 1). For all other possible values of $\cos \delta$, the $H_{c2}$ curve lies between these two extremes. The limit $\cos \delta = 1$ is unlikely since this implies that the density of states of one of the two bands vanishes. However, if the elements of the pairing interaction $V_{a,b}$ in Eq. 5 are different in magnitude from each other, then a large $ql_H$ can still arise for $\cos \delta = 0$.

Comparing our result with the $H_{c2}$-measurement by Yasuda et al.\textsuperscript{8} for CePt$_3$Si, we find that only taking the effect of the spin-orbit coupling into account would not account for the relatively large value of the in-plane $H_{c2} \approx 2.8T$ at $T = 0$. Here, paramagnetic limiting should reduce the value to below 2 T. We can, however, explain the increased $H_{c2}$ by including the helicity.

We have also examined the behavior of the Abrikosov parameter $\beta_{\lambda} = (\langle \Psi(R) \rangle^2/\langle |\Psi(R)|^2 \rangle)^2$ in connection with the possible vortex lattice structures. We find a possible structural transition from a stretched hexagonal lattice at high temperatures to a stretched square lattice at low temperatures. The origin of this transition is related to the two-dimensional inhomogeneous state discussed in Refs. 15-19. Note that the helical order discussed above is distinct from that discussed in these works. The physics discussed in Refs. 15-19 does not play a significant role in CePt$_3$Si because the value of $\alpha_M$ is too small. However, if $\alpha_M >> 1$ then the vortex physics becomes very exotic.

We have not discussed the direct experimental verification of the helical phase. Since helicity of the order parameter is related to its phase, an interference experiment based on the Josephson effect would provide the most reliable test. Here we propose to consider a Josephson junction between two thin film superconductors (Fig. 2), one (1) with and the other (2) without inversion symmetry (for CePt$_3$Si the c-axis is perpendicular to the film).
For a magnetic field applied in the plane of the film perpendicular to the junction and with the superconductor (2) is oriented so that the helicity \( q \) is perpendicular to the field; we find this gives rise to an interference effect analogous to the standard Fraunhofer pattern. For this experiment, the film must be sufficiently thin that the magnetic field and the magnitude of the order parameter are spatially uniform.

To illustrate this, consider the following free energy of the junction

\[
H_J = -t \int dx \Psi_1^*(R) \Psi_2(R) + c.c.
\]

where the integral is along the junction. The resulting Josephson current is

\[
I_J = Im \left[ t \int dx \Psi_1^*(R) \Psi_2(R) \right]
\]

Setting the junction length equal to \( 2L \), and integrating yields a maximum Josephson current of

\[
I_J = 2t|\Psi_1^0||\Psi_2^0| \sin(qL)|/qL|
\]

This, combined with the result of the microscopic theory near \( T_c \) (for an isotropic interaction) that \( qL = 2.4 \cos \delta \alpha_{3/2} H_{c2} L / \Phi_0 \) (where \( \xi_0 = 0.18 v_F / T_c \)) demonstrates that the Josephson current will display an interference pattern for a field perpendicular to the junction. Note that in the usual case the Fraunhofer pattern would be observed for a magnetic field perpendicular to the thin film. Furthermore, for a sufficiently large in-plane field, so that \( |qL| >> 1 \) (which implies \( I_J \approx 0 \)), the arguments of Ref. 21 imply that the application of an additional magnetic field along the surface normal will lead to an asymmetric Fraunhofer pattern.

A less direct probe of the helical order is to look for the related transverse magnetization that appears in Eq. 9. There are two situations for which this can be observed. The first is in a thin film with a supercurrent flowing along \( x \) and a surface normal along \( y \). In this case a magnetization will exist along \( y \) (normal to the film). This situation is a generalization of an experiment originally proposed by Edelstein. We estimate \( |m| = \frac{\mu_B v_s}{4 \pi} \cos \delta \eta L v_F / v_F \sim 0.02 \) Gauss assuming \( v_s / v_F = 2 \times 10^{-4} \), \( \cos \delta = 1/3 \), and \( n_s = 1 \times 10^2 \) m\(^{-3} \). The second is in the vortex lattice phase for a field applied along the c-axis. In this case, a calculation valid near \( H_{c2} \) gives \( m = \frac{m_r}{\xi} n \times J_0 \), where \( J_0 \) is the usual supercurrent for the Abrikosov vortex lattice. Near the vortex core, \( m \) is directed radially outward, perpendicular to the applied field.

We have considered the role of magnetic fields on the non-centrosymmetric superconductor CePt\(_3\)Si. Using a two-band theory with a Rashba spin-orbit interaction, we have shown that the upper critical field for the field along the c-axis behaves as if it would in a conventional superconductor independent of the paramagnetic (Zeman) field. We have further shown that while there is a paramagnetic limiting effect for magnetic fields applied in the basal plane, this effect can be strongly reduced by the appearance of a helical order. Our theory agrees with the experimental measurements of \( H_{c2} \), despite a relatively strong Zeeman field, provided this helical order exists. Finally, we have proposed a Josephson junction experiment that can unambiguously identify the helical order and discussed the appearance of a transverse magnetization related to the helical order.

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1. E. Bauer et al., Phys. Rev. Lett. 92, 027003 (2004).
2. P.A. Frigeri, D.F. Agterberg, A. Koga, and M. Sigrist, Phys. Rev. Lett. 92, 097001 (2004).
3. K.V. Samokhin, E.S. Zijlstra, and S. Bose, Phys. Rev. B 69, 094514 (2004).
4. S.S. Saxena and P. Monthoux, Nature 427, 799 (2004).
5. I.A. Sergienko and S.H. Cunroe, cond-mat/0406003.
6. V.P. Mineev, cond-mat/0406371.
7. K.V. Samokhin, cond-mat/0404407.
8. T. Yasuda et al., J. Phys. Soc. Jpn. 73, 1657 (2004).
9. M. Yogi et al., Phys. Rev. Lett. 93, 027003 (2004).
10. P.W. Anderson, J. Phys. Chem. Solids 11, 26 (1959).
11. P.W. Anderson, Phys. Rev. B 30, 4000 (1984).
12. L.N. Bulaevskii, A.A. Guseinov and A.I. Rusinov, Sov. Phys. JETP 44, 1243 (1976).
13. L.P. Gor’kov and E.I. Rashba, Phys. Rev. Lett. 87, 037004-1 (2001).
14. E. Helfand and N.R. Werthamer, Phys. Rev. Lett. 13, 686 (1964).
15. V.P. Mineev and K.V. Samokhin, JETP 78, 401 (1994), (Zh. Eksp. Teor. Fiz. 105, 747 (1994)).
16. V.M. Edelstein, Sov. Phys. JETP 68, 1244 (1989).
17. D. F. Agterberg, Physica C 387, 13 (2003).
18. O. V. Dimitrova and M. V. Feigelman, Pisma Zh. Eksp.
19. V. Barzykin and L.P. Gor’kov, Phys. Rev. Lett. 89, 227002 (2002).
20. H. Adachi and R. Ikeda, Phys. Rev. B 68, 184510 (2003).
21. K. Yang and D.F. Agterberg, Phys. Rev. Lett. 84, 4970 (2000).
22. V.M. Edelstein, Phys. Rev. Lett. 75, 2004 (1995).