Magnetic Properties in Non-centrosymmetric Superconductors with and without Antiferromagnetic Order

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The paramagnetic properties in non-centrosymmetric superconductors with and without antiferromagnetic (AFM) order are investigated with focus on the heavy Fermion superconductors, CePt\(_3\)Si, CeRhSi\(_3\) and CeIrSi\(_3\). First, we investigate the spin susceptibility in the linear response regime and elucidate the role of AFM order. The spin susceptibility at \(T = 0\) is independent of the pairing symmetry and increases in the AFM state. Second, the non-linear response to the magnetic field are investigated on the basis of an effective model for CePt\(_3\)Si which may be also applicable to CeRhSi\(_3\) and CeIrSi\(_3\). The role of antisymmetric spin-orbit coupling (ASOC), helical superconductivity, anisotropic Fermi surfaces and AFM order are examined in the dominantly s-, p- and d-wave states. We emphasize the qualitatively important role of the mixing of superconducting (SC) order parameters in the p-wave state which enhances the spin susceptibility and suppresses paramagnetic depairing effect in a significant way. Therefore, the dominantly p-wave superconductivity admixed with the s-wave order parameter is consistent with the paramagnetic properties of CePt\(_3\)Si at ambient pressure. We propose some experiments which can elucidate the novel pairing states in CePt\(_3\)Si as well as CeRhSi\(_3\) and CeIrSi\(_3\).

KEYWORDS: Superconductivity without inversion center; antiferromagnetic superconductor; Pauli paramagnetic effect; spin susceptibility

1. Introduction

Since the discovery of superconductivity in the non-centrosymmetric heavy Fermion compound CePt\(_3\)Si\(^1,2\) superconductivity in materials without inversion center is attracting growing interest. Many new non-centrosymmetric superconductors (NCSC) with unusual properties have been identified among heavy fermion systems such as UIr\(^3\), CeRhSi\(_3\)\(^4,5\), CeIrSi\(_3\)\(^6,7\), CeCoGe\(_3\)\(^8\) and others like Li\(_2\)Pd\(_3\)Pt\(_3\)\(_-\)B\(_9\)\(^9\), Y\(_2\)C\(_3\)\(_10\), Rh\(_2\)Ga\(_9\), Ir\(_2\)Ga\(_9\)\(_-\)\(^11,12\), Mg\(_{\text{16}}\)Ir\(_{\text{19}}\)B\(_{\text{16}}\)\(_{13}\), Re\(_3\)W\(_{\text{14}}\) and some organic materials.\(^15\) The aspects of missing inversion symmetry are also of great interest for other materials. For example, the spin Hall effect in the semiconductor\(^16\) and the helical magnetism in MnSi\(^17\) are very active research fields.

NCSC adds several unusual aspects to the properties of superconductivity. One immediate consequence of non-centrosymmetry is the necessity for an extended classification scheme of Cooper pairing states, as parity is not available as a distinguishing symmetry. Using the traditional scheme the SC states here may be represented as a mixture of pairing states of even and odd parity, or, equivalently, their spin configuration is a superposition of a singlet and a triplet component. This is a consequence of the presence of antisymmetric spin-orbit coupling (ASOC) in non-centrosymmetric materials.\(^18\) Recent theoretical studies led to the discussion of various intriguing properties which could appear in NCSC, such as the magneto-electric effect\(^18-22\) the unusual anisotropic spin susceptibility,\(^18,20,22-28\) the occurrence of an anomalous coherence effect in NMR 1/\(T_1\)\(_c\)\(^21,29\) the unusual origin of nodes in the SC gap,\(^27,29-32\) the realization of the helical SC phase,\(^33-38\) the possible appearance of Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) state at zero magnetic field,\(^39\) de Haas-van Alphen effect,\(^40\) various novel impurity effects,\(^41-43\) and vortex core states\(^44\) and unconventional features in quasiparticle tunneling and Josephson effect.\(^45-52\)

The non-centrosymmetric heavy fermion superconductors, e.g. CePt\(_3\)Si, UIr, CeRhSi\(_3\), CeIrSi\(_3\) and CeCoGe\(_3\) are of particular interests because the Cooper pairing is most likely unconventional (non-s-wave) due to the strong electron correlation. Although many studies have been devoted to this topics, there is no consensus on the symmetry of pairing in these compounds so far. The symmetry of Cooper pairs may be determined by the paramagnetic properties such as the spin susceptibility below \(T_c\).

In centrosymmetric superconductor, the spin susceptibility is a distinguishing feature for the spin configuration of the pairing state, as it decreases below \(T_c\) for the spin singlet superconductor and remains constant in the case of spin triplet pairing, if the magnetic field is perpendicular to the \(d\)-vector (parallel to the equal-spin direction).\(^53,54\) The measurements of the Knight shift which is proportional to the spin susceptibility have played an important role for the identification of SC state in various compounds.\(^55\) For superconductors with very high \(H_{c2}\) probing effects of paramagnetic limiting can give also insight into the pairing symmetry and has been applied in connection with NCSC. However, the response to the magnetic field is not so straightforward in non-centrosymmetric systems.
As mentioned above, spin singlet and triplet components are mixed in the pairing state. Furthermore the band splitting induced by the ASOC affects the magnetic properties. Therefore, it is necessary to clarify the magnetic properties very carefully before drawing strong conclusions. In this context also the influence of AFM order on the (magnetic) properties of the SC phase is an important point to investigate, since all presently known non-centrosymmetric heavy fermion superconductors, i.e. CePt$_3$Si, UIr, CeRhSi$_3$, CeIrSi$_3$ and CeCoGe$_3$, coexist with the magnetism. In CePt$_3$Si at ambient pressure, superconductivity ($T_c = 0.75$K) coexists with AFM order ($T_N = 2.2$K). The AFM order can be suppressed by pressure and vanishing at the critical value of $P \sim 0.6$GPa. The SC phase is more robust and a purely SC phase exists beyond the critical pressure, ($P > 0.6$GPa). The AFM order of $\sim 6$GPa). The AFM order is quantitatively important for the magnetic properties very carefully before drawing conclusions.

The non-linear response to the magnetic field is important when the magnetic field is comparable to or larger than the normal state value at $T = 0$, in absence of AFM order. The influence of helicity (Cooper pairs possess a finite momentum) in NCSC on the behavior of the susceptibility turns out to be negligible. On the other hand, the folding of Brillouin zone due to the AFM order significantly affects the spin susceptibility in the SC phase. The spin susceptibility remains nearly constant through the critical value of $P \sim 0.6$GPa. The SC phase is more robust and a purely SC phase exists beyond the critical pressure, ($P > 0.6$GPa). The AFM order of $\sim 6$GPa). The AFM order is quantitatively important for the magnetic properties very carefully before drawing conclusions.

In this paper we investigate the linear as well as the non-linear response regime of the NCSC in a magnetic field with the aim to provide guidelines to identify the pairing symmetry based on magnetic properties. Before going into details we briefly summarize the main conclusions of our study. It is known that in the linear response regime the paramagnetic properties are universal i.e. the spin susceptibility is independent of the pairing symmetry. In the presence of Rashba-type ASOC, the spin susceptibility along the $c$-axis is constant through $T_c$ while it decreases along the $ab$-plane to half of the normal state value at $T = 0$, in absence of AFM order. The influence of helicity (Cooper pairs possess a finite momentum) in NCSC on the behavior of the susceptibility turns out to be negligible. On the other hand, the folding of Brillouin zone due to the AFM order significantly affects the spin susceptibility in the SC phase. The spin susceptibility remains nearly constant through the critical value of $P \sim 0.6$GPa. The SC phase is more robust and a purely SC phase exists beyond the critical pressure, ($P > 0.6$GPa). The AFM order of $\sim 6$GPa). The AFM order is quantitatively important for the magnetic properties very carefully before drawing conclusions.

The non-linear response to the magnetic field is important when the magnetic field is comparable to or higher than the standard paramagnetic limiting field $H_P \sim 1.2k_BT_c/\mu_B$. It should be noted that most of the experimental studies, such as the Knight shift and critical magnetic field $H_{c2}$, have been carried out in the non-linear response region. The pairing state in NCSC can be identified by the measurements in the non-linear response regime because the paramagnetic properties depend on the pairing symmetry in contrast to the situation in the linear response regime. We show that the critical magnetic field $H_{c2}$ along the $ab$-plane is significantly enhanced in the non-linear response regime by the formation of helical SC state. This enhancement coincides with the non-linear increase of the helicity of the SC order parameter. $H_{c2}$ further rises for the dominantly $p$-wave state owing to the mixing of SC order parameters. These effects, namely (i) the formation of the helical SC state and (ii) the mixing of SC order parameters, are quantitatively important for anisotropic Fermi surfaces. AFM order significantly enhances the effect (ii) and also boosts $H_{c2}$. In this case, the spin susceptibility remains nearly constant through $T_c$. On the other hand, these effects are negligible in the dominantly spin singlet pairing state. Since the influence of AFM order is quantitatively important, the paramagnetic properties of the SC phase in the AFM state provide a means to distinguish between pairing states with dominant spin triplet and singlet component.

Among the non-centrosymmetric heavy fermion superconductors, CePt$_3$Si has been investigated in most detail because the superconductivity exists at ambient pressure while others require substantial pressure to become superconducting. Therefore, we pay particular attention to the situation in CePt$_3$Si, and discuss the pairing symmetry by comparing the experimental results with our theoretical results. The paramagnetic properties of CePt$_3$Si look puzzling at first sight because the experimental results are incompatible with the theoretical results within the linear response theory and without taking into account the AFM order. In our present study we show that the experimental results are consistent with the theoretical results for the dominantly $p$-wave state by taking into account the AFM order as well as the non-linear response to the magnetic field.

Moreover we propose further test experiments which could strengthen our conclusions. First, the influence of AFM order can be examined by the pressure which suppresses the AFM order. Second, the 2-fold anisotropy in the $ab$-plane arises from the AFM order and the anisotropy is qualitatively different between the dominantly $p$-wave, inter-plane $d$-wave and intra-plane $s$- or $d$-wave states. Future experimental studies of these kind could help identify the pairing symmetry in CePt$_3$Si, CeRhSi$_3$, CeIrSi$_3$ and CeCoGe$_3$.

The paper is organized as follows. In §2 we summarize the linear response theory for the paramagnetic properties in NCSC. In §3 we introduce the effective model for CePt$_3$Si which could be also applied to CeRhSi$_3$, CeIrSi$_3$ and CeCoGe$_3$. The paramagnetic properties in the magnetic field along the $ab$-plane are investigated in §4 and §5. The non-linear response to the magnetic field for the dominantly $s$-wave state is investigated in §4. In §5, which is the main part of this paper, we show the magnetic properties in the dominantly $p$-wave state. The influences of the helical superconductivity, anisotropic Fermi surface and AFM order are elucidated. The pairing symmetry of CePt$_3$Si is discussed in §6 by comparing the experimental results with our theoretical results. Some test experiments are proposed for CePt$_3$Si, CeRhSi$_3$ and CeIrSi$_3$ in §7. In §8, nature of the helical SC state is investigated in details. We show the crossover from the helical SC state with long wave length to that with short wave length. These results are summarized and some discussions are given in §9.
2. Linear Response Theory

In this section we investigate the linear response regime of the NCSC in a magnetic field, and study the magnetic properties in the paramagnetic (PM) and in the AFM phase. The latter we consider both for the case of a centrosymmetric and a non-centrosymmetric system.

2.1 General spin susceptibility

In a first step we derive a general expression for the spin susceptibility in the SC state on the basis of the extended BCS Hamiltonian, given by

\[ H = H_b + H_{SO} + H_{AF} + H_{\Delta}, \]

\[ H_b = \sum_{\tilde{k}, s} \varepsilon(\tilde{k}) c_{\tilde{k}, s}^\dagger c_{\tilde{k}, s}, \tag{2} \]

\[ H_{SO} = \alpha \sum_{\tilde{k}} \hat{g}(\tilde{k}) \cdot \hat{S}(\tilde{k}), \tag{3} \]

\[ H_{AF} = -\sum_{\tilde{k}} \hat{h}_Q \cdot \hat{S}_Q(\tilde{k}), \tag{4} \]

\[ H_{\Delta} = -\sum_{s, s', \tilde{k}} \left[ \Delta_{1, s', s}(\tilde{k}) c_{\tilde{k}, s'}^\dagger c_{\tilde{k}, s} + \Delta_{2, s', s}(\tilde{k}) c_{\tilde{k} + \tilde{Q}, s'}^\dagger c_{\tilde{k}, s} + h.c. \right], \tag{5} \]

where \( \tilde{k}_z = \tilde{k} \pm \hat{q}_H/2 \), \( \hat{S}(\tilde{k}) = \sum_{s' s} s_{s'} c_{\tilde{k}, s'}^\dagger c_{\tilde{k}, s} \) and \( \hat{S}_Q(\tilde{k}) = \sum_{s s'} s_{s'} c_{\tilde{k} + \tilde{Q}, s'}^\dagger c_{\tilde{k}, s} \). Here \( \hat{q}_H \) is the total momentum of Cooper pairs. Note that \( \hat{q}_H \) is zero in the usual BCS state while that is finite in the helical SC state.\(^{33-38} \) NCSC the helical SC state can be realized under magnetic field above \( H_c \). We consider a tetragonal crystal lattice and assign the \( x, y, z \)-axis to \( a, b, c \)-axis, respectively.

The first term in eq. (1) describes the dispersion relation without ASOC and AFM order. In this subsection we do not identify the specific dispersion of the electrons and assume \( \varepsilon(\tilde{k}) \) as general.

The second term \( H_{SO} \) describes the ASOC due to the lack of inversion symmetry. This term preserves time reversal symmetry, if the \( g \)-vector is odd in \( \tilde{k} \), i.e. \( \hat{g}(\tilde{k}) = -\hat{g}(\tilde{k}) \). We consider a Rashba-type spin-orbit coupling\(^{71} \) as is realized in CePt\(_3\)Si, CeRhSi\(_3\), CeIrSi\(_3\) and CeCoGe\(_3\).\(^{72,74} \) Because the detailed momentum dependence of \( \hat{g}(\tilde{k}) \) is unknown, we express it in terms of velocities \( \hat{v}(\tilde{k}) = \partial \varepsilon(\tilde{k})/\partial \tilde{k} : \hat{g}(\tilde{k}) = (\hat{v}_y(\tilde{k}), \hat{v}_x(\tilde{k}), 0)/\hat{v} \). This choice at least preserves the correct periodicity in \( \tilde{k} \)-space. The detailed form of the \( g \)-vector is arbitrary important in the following. We normalize the \( g \)-vector \( \hat{g}(\tilde{k}) \) by the average velocity \( \hat{v} = [\hat{v}^2 = \frac{1}{2} \sum k v_y(\tilde{k})^2 + v_x(\tilde{k})^2] \) so that the coupling constant \( \alpha \) has the dimension of energy. We assume the relation \( |\Delta_{1, s', s}(\tilde{k})| \ll |\alpha| \ll \varepsilon_F \) throughout this paper (\( \varepsilon_F \) is the Fermi energy). This relation is valid for the most of NCSC such as CePt\(_3\)Si, UIr, CeRhSi\(_3\), CeIrSi\(_3\) and CeCoGe\(_3\).

The third term \( H_{AF} \) is taken into account to investigate the role of AFM order which enters through the staggered field \( \hat{h}_Q \). We focus on A-type AFM order, i.e. ferromagnetic sheets in the \( ab \)-plane are staggered along the \( c \)-axis, giving rise to \( \hat{Q} = (0, 0, \pi) \). This spin structure is realized in CePt\(_3\)Si\(^{77} \) as well as the centrosymmetric superconductor UPd\(_2\)Al\(_5\).\(^{72,74} \) where the magnetic moments are aligned in the \( ab \)-plane. A different AFM state has been reported for CeRhSi\(_3\)\(^{74} \) and the magnetic structure is not clearly identified for CeIrSi\(_3\) so far. However, the qualitative role of AFM order can be captured by \( \hat{Q} = (0, 0, \pi) \) in the simple cases.

The last term \( H_{\Delta} \) describes the mean field term of the SC order. The order parameter is given by \( \Delta_{1, s', s}(\tilde{k}) \) and \( \Delta_{2, s', s}(\tilde{k}) \). The second component \( \Delta_{2, s', s}(\tilde{k}) \) only appears in the case of superconductivity coexisting with AFM order \( (\Delta_{2, s', s}(\tilde{k}) = 0 \text{ for } \hat{h}_Q = 0) \). The order parameter has both the spin singlet and triplet components owing to the ASOC.

It is more transparent for the following discussion to consider the order parameter in the band basis because the superconductivity is mainly induced by the intra-band Cooper pairing when \( |\Delta| \ll |\alpha| \). Ignoring the order parameters describing the inter-band pairing, we obtain the simplified Hamiltonian as,

\[ H_{\text{band}} = \sum_{\gamma=1}^{4} \sum_{\tilde{k}} \varepsilon(\tilde{k}) a_{\gamma, \tilde{k}}^\dagger a_{\gamma, \tilde{k}} + h.c. \]
The normal and anomalous Green functions are expressed in the band basis as,
\[ G_{\alpha}(\vec{k}, \omega_n) = (i\omega_n + e_{\alpha}(-\vec{k})) / A_{\alpha}(\vec{k}, \omega_n), \]
\[ F_{\alpha}(\vec{k}, \omega_n) = -\Delta_{\alpha}(\vec{k}) / A_{\alpha}(\vec{k}, \omega_n), \]
with
\[ A_{\alpha}(\vec{k}, \omega_n) = (i\omega_n - e_{\alpha}(\vec{k})) (i\omega_n + e_{\alpha}(-\vec{k})) - |\Delta_{\alpha}(\vec{k})|^2, \]
where \( \omega_n = (2n + 1)\pi T \) is the Matsubara frequency and \( T \) is the temperature.

We decompose the uniform spin susceptibility into the Pauli part and Van-Vleck part,
\[ \chi_{\mu\nu} = \chi^P_{\mu\nu} + \chi^V_{\mu\nu}. \]
The Pauli susceptibility \( \chi^P_{\mu\nu} \) arises from the intra-band scattering while the inter-band scattering gives rise to the Van-Vleck susceptibility (VVS) \( \chi^V_{\mu\nu} \). In the following we assume the staggered moments along the principal axis, namely \( \vec{h}_Q \parallel \hat{x}, \hat{y} \) or \( \hat{z} \). Following the Appendix A, the Pauli susceptibility and VVS are expressed as,
\[ \chi^P_{\mu\nu} = -\lim_{\vec{q} \to 0} \lim_{\Delta_{\mu\nu} \to 0} \sum_{\gamma, \vec{k}} A_{\gamma\gamma}(\vec{k}) \times [G_{\gamma}(k + q)G_{\gamma}(k) \pm F_{\gamma}(k + q)F_{\gamma}(k)], \]
and
\[ \chi^V_{\mu\nu} = \sum_{\gamma \gamma' \delta \vec{k}} A_{\gamma\gamma'}(\vec{k}) f(\varepsilon_{\gamma}(\vec{k})) - f(\varepsilon_{\gamma'}(\vec{k})) / \varepsilon_{\gamma}(\vec{k}) - \varepsilon_{\gamma'}(\vec{k}), \]
respectively. The sign in eq. (15) is + for \( \mu = x, y \) and − for \( \mu = z \). We define \( A_{\gamma\gamma'}(\vec{k}) = S_{\gamma\gamma'}(\vec{k}, \vec{k}) S_{\gamma\gamma'}(\vec{k}, \vec{k}) \) where \( S_{\gamma\gamma'}(\vec{k} + q, \vec{k}) \) is the spin operator in the band basis,
\[ \check{S}\mu(\vec{k} + q, \vec{k}) = \check{U}(\vec{k} + \vec{Q}) \check{S} \check{U}(\vec{k}), \]
with
\[ \check{S}\mu = \begin{pmatrix} \hat{\sigma}(\mu) & 0 \\ 0 & \hat{\sigma}(\mu) \end{pmatrix}. \]

The expression of Pauli susceptibility eq. (15) is equivalent to the spin susceptibility in a multi-band system. The sign + and − in eq. (15) correspond to the centrosymmetric superconductor with spin singlet pairing and that with spin triplet pairing for \( d \perp \hat{H} \), respectively. Thus, the Pauli susceptibility of NCSC decreases in the \( ab \)-plane below \( T_c \) while that is constant for the magnetic field along the \( c \)-axis.

It should be noted that the VVS has a temperature dependence above \( T_c \) which is similar to that of Pauli susceptibility, because the ASOC is much smaller than the Fermi energy (\( |\alpha| \ll \varepsilon_F \)). Therefore, the VVS in eq. (14) should be included in the spin part of magnetic susceptibility which is extracted by the K-\( \chi \) plot. In this sense, the VVS, arising from the band splitting due to the ASOC, is quite different from the better known VVS coming from the orbital degrees of freedom. Note that both VVS are not affected by the superconductivity when \( T_c \ll |\alpha| \).

If the order parameter is spatially uniform, namely \( \vec{g}_Q = 0 \), the Pauli susceptibility is described by the momentum dependent Yoshida function as,
\[ \chi^P_{\mu\nu} = \sum_{\gamma} \int d\vec{k}_F A_{\gamma\gamma}(\vec{k}_F) Y(\Delta_{\gamma}(\vec{k}_F), T) / v_{\gamma}(\vec{k}_F), \]
for \( \mu = x, y \), and
\[ \chi^V_{\mu\nu} = \sum_{\gamma} \int d\vec{k}_F A_{\gamma\gamma}(\vec{k}_F) / v_{\gamma}(\vec{k}_F), \]
where \( \int d\vec{k}_F \) is the integral on the Fermi surface, and \( v_{\gamma}(\vec{k}_F) \) is the Fermi velocity of \( \gamma \)-th band. The Yoshida function is defined as,
\[ Y(\Delta, T) = -\int d\varepsilon f'(\sqrt{\varepsilon^2 + \Delta^2}), \]
where \( f'(E) = df / dE \) is the Fermi distribution function. Since \( Y(\Delta, 0) = 0 \) and \( Y(0, T) = 1 \), we obtain \( \chi^P_{\mu\nu}(T = 0) = \chi^V_{\mu\nu} \) for \( \mu = x, y \) and \( \chi_{xz}(T = 0) = \chi_{zx} + \chi^P_{xz}(T = T_c) = \chi_{zx}(T = T_c) \). Thus, the residual spin susceptibility along \( ab \)-plane is given by the VVS alone, while for fields parallel to the \( c \)-axis both the Pauli and Van-Vleck susceptibility contribute. It should be noticed that the spin susceptibility at \( T = 0 \) is independent of the pairing symmetry. In this sense the spin susceptibility is universal in the linear response regime when the system lacks the inversion symmetry.

2.2 PM state

We concentrate now on the uniform state (\( \vec{g}_Q = 0 \)) to investigate the residual spin susceptibility \( \chi_{\mu\nu} \) at \( T = 0 \) for \( \mu = x, y \). The helical SC state with \( \vec{g}_Q \neq 0 \) will be discussed later in §8. In the PM state we set \( \vec{h}_Q = 0 \) and assign the four bands as \( e_{1,2}(k) = (\varepsilon(k) + \alpha|\vec{g}(k)|) \), \( e_{3,4}(k) = (\varepsilon(k) + \vec{Q}) \pm \alpha|\vec{g}(k) + \vec{Q}|| \) so that we can express the unitary matrix as,
\[ \check{U}(\vec{k}) = \begin{pmatrix} \check{U}_2(\vec{k}) & 0 \\ 0 & \check{U}_2(\vec{k} + \vec{Q}) \end{pmatrix}, \]
with
\[ \check{U}_2(\vec{k}) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \check{g}_x(\vec{k}) + i\check{g}_y(\vec{k}) & -\check{g}_x(\vec{k}) - i\check{g}_y(\vec{k}) \end{pmatrix}\]
with \( \check{g}_\mu(\vec{k}) = g_\mu(\vec{k}) / |\vec{g}(\vec{k})| \). The matrix element of spin operator is obtained as, \( S^x_{11}(\vec{k}, \vec{k}) = -S^x_{12}(\vec{k}, \vec{k}) = \check{g}_x(\vec{k}) \) and \( S^x_{22}(\vec{k}, \vec{k}) = -S^x_{44}(\vec{k}, \vec{k}) = \check{g}_x(\vec{k} + \vec{Q}) \) for \( \mu = x, y \) while \( S^x_{11}(\vec{k}, \vec{k}) = 0 \). We then find \( \chi_{xx} = \chi_{xx}^P + \chi_{xx}^V = \rho + O(\alpha^2 / \varepsilon_F^2) \) in the normal state, the residual spin susceptibility at \( T = 0 \) is obtained as,
\[ \chi_{xx}(T = 0) = \chi_{xx} = \chi_{xx}(T = T_c) / 2 + O(\alpha^2 / \varepsilon_F^2). \]
Thus, the spin susceptibility in the \( ab \)-plane at \( T = 0 \) is half of the normal state value in the limit \( |\alpha| \ll \varepsilon_F \). Qualitatively the same result has been obtained in Refs. 18,20,22-28. Fujimoto has shown that the VVS increases when the DOS has strong asymmetry and \( |\alpha| \) is moderate. However, the \( 3 \)-band of CePt_3Si which we will investigate later does not satisfy this condition.
Since the spin susceptibility decreases below $T_c$ for the magnetic field along the $ab$-plane, the paramagnetic depairing effect of $H_{c2}$ should be observed in NCSC with Rashba-type spin-orbit coupling. This is consistent with the recent observation of the paramagnetic depairing effect in CeRhSi$_3$ and CeIrSi$_3$ under high pressure where the AFM order is suppressed. However, this is not the case in CePt$_3$Si at ambient pressure (within the AFM phase). This observation leads us to study the influence of AFM order in the following part.

## 2.3 AFM state with inversion symmetry

In order to clarify the influence of AFM order, we first investigate the spin susceptibility in the SC state with inversion symmetry for $\vec{H} \neq 0$. Owing to the inversion symmetry, the residual spin susceptibility depends on the pairing symmetry in the usual way. Here we discuss the spin singlet pairing state while the spin susceptibility is constant through $T_c$ in the spin triplet pairing state. The spin susceptibility consists of the Pauli part and Van-Vleck part as in the spin susceptibility consists of the Pauli part and Van-Vleck part in the usual way. Here we discuss the spin susceptibility in the SC state in the normal state is little affected.

The presence of quasi-two dimensional Fermi surface is also expected in CeRhSi$_3$. The large residual spin susceptibility, although the multiorbital effect is another possible origin. This is consistent with the large $H_{c2}$ which exceeds the standard paramagnetic limit.

At this point we can discuss the role of the band structure. According to eq. (26), the Pauli part of the spin susceptibility is small for the magnetic field $\vec{H} \perp \vec{h}_Q$, if the quasiparticle dispersion is quasi-two dimensional and $\varepsilon_-(\vec{k})$ is small. Although the $\beta$-band of CePt$_3$Si has a three dimensional Fermi surface, the band dispersion is weak along the $k_z$-axis according to the result of band calculation. This means that the AFM order significantly would affect the SC state in this band of CePt$_3$Si. The presence of quasi-two dimensional Fermi surface is also expected in CeRhSi$_3$.

There are cases where AFM order plays indeed an important role in a centrosymmetric material. For example, UPd$_2$Al$_3$ is a spin singlet superconductor with $T_c = 2K$ which coexists with the AFM order. The AFM state has a high Néel temperature of $T_N = 14K$ and a large staggered magnetic moment, $m = 0.85\mu_B$. This moment is directed to the $ab$-plane of tetragonal lattice and $\hat{Q} = (0,0,\pi)$. This is the same spin structure as CePt$_3$Si. NMR measurements show the decrease of Knight shift below $T_c$ with a large residual part.

The VVS arising from the AFM order may induce the large residual spin susceptibility, although the multi-orbital effect is another possible origin. This is consistent with the large $H_{c2}$ which exceeds the standard paramagnetic limit.

## 2.4 AFM state without inversion symmetry

The result in §2.3 implies that the AFM order enhances the Van-Vleck part of spin susceptibility in the...
non-centrosymmetric system for the magnetic field perpendicular to the AFM moment. We have shown the results for the spin susceptibility along the \(a\) and \(b\) axes by assuming the dispersion relation eqs. (27), (28), \(\alpha = 0.3\) and \(\vec{h}_Q \parallel \vec{x}\) to describe the electronic structure of CePt\(_3\)Si below \(T_X\) (Fig. 4 of Ref. 27). For fields \(\vec{H} \perp \vec{h}_Q\) the normal state and SC state susceptibility merge for increasing staggered moment, suggesting a diminishing of the reduction of the spin susceptibility in the SC state. On the other hand, the behavior is opposite for \(\vec{H} \parallel \vec{h}_Q\). Thus, a remarkable 2-fold anisotropy is expected in the spin susceptibility below \(T_c\) even if the anisotropy is weak in the normal state. The condition \(\vec{H} \perp \vec{h}_Q\) is generally favored because the magnetization energy is maximally gained for the field direction with largest spin susceptibility. However, the meta-stable state \(\vec{H} \parallel \vec{h}_Q\) can be realized in the weak magnetic field which is smaller than the anisotropy energy of AFM moment.

The role of AFM order is suppressed by increasing the ASOC. We have confirmed that \(\chi_{\perp}^H\) in the SC state is decreased by increasing \(\alpha\) when \(\vec{h}_Q \parallel \vec{x}\). The AFM order plays a quantitatively important role when the ASOC is much smaller than the Fermi energy.

If the AFM moment is parallel to the \(c\)-axis as in CeCoGe\(_3\),\(^8\) the spin susceptibility along both \(a\) and \(b\) axes is increased in the SC state by the AFM order, while that along the \(c\)-axis is not affected.

3. Effective Model for CePt\(_3\)Si, CeRhSi\(_3\) and CeIrSi\(_3\)

In preparation for the discussion of the non-linear response to the magnetic field we will introduce here an effective model for CePt\(_3\)Si, CeRhSi\(_3\) and CeIrSi\(_3\). This is important as we will show that the non-linear spin susceptibility significantly depends on the symmetry of order parameter in contrast to the universal spin susceptibility in the linear response theory (see §2.1). In particular, we point out the strong non-linearity in the pairing state with dominant \(p\)-wave character.

We analyze the following effective model,

\[
H = H_0 + H_{SO} + H_{AF} + H_Z + H_1, \tag{29}
\]

\[
H_Z = -\sum_{\vec{k}} \vec{h} \cdot \vec{S}(\vec{k}), \tag{30}
\]

\[
H_1 = U \sum_i n_{i,\uparrow} n_{i,\downarrow} + (V - J/4) \sum_{<i,j>} n_i n_j
+ J \sum_{<i,j>} \left[ \vec{S}_i \cdot \vec{S}_j - 2S_i^x S_j^x \right] \tag{31}
\]

\[
= \frac{1}{2} \sum_{\vec{k},\vec{k}',\vec{q},\vec{q}',\pm} \left[ VC(\vec{k} - \vec{k}')c^\dagger_{\vec{k},s}c^\dagger_{\vec{k}',s} c_{\vec{k}',\pm,s} c_{\vec{k},\pm,s} + \right]
+ C(\vec{k} - \vec{k}')c^\dagger_{\vec{k},s}c^\dagger_{\vec{k}',s} c_{\vec{k}',s} c_{\vec{k},s} - \frac{1}{2} C(\vec{k} - \vec{k}')c^\dagger_{\vec{k},s}c^\dagger_{\vec{k}',s} c_{\vec{k}',s} c_{\vec{k},s}, \tag{32}
\]

where \(n_{i,s}\) is the electron number at the site \(i\) with spin \(s\), \(n_i = n_{i,\uparrow} + n_{i,\downarrow}\), \(\vec{s} = (-s)\) and \(C(\vec{k}) = 2(\cos k_x + \cos k_y)\). The spin operator in the real space basis is defined as \(\vec{S}_i = \sum_{s,s'} \vec{e}_{ss'}^i c^\dagger_{i,s} c_{i,s'}\). The bracket \(< i, j >\) denotes the summation for the nearest neighbor sites in the \(ab\)-plane, namely \(j = i \pm \vec{a}\) or \(j = i \pm \vec{b}\) with \(\vec{a}\) and \(\vec{b}\) the unit vectors along the \(a\) and \(b\)-axis, respectively.

The first three terms in eq. (29) have been defined earlier in eqs. (2-4). For the dispersion relation, we adopt the tight-binding model eq. (27) with using the parameter set eq. (28) and \(\alpha = 0.3\), reproducing the \(\beta\)-band of CePt\(_3\)Si.\(^79\)–\(^81\) We choose the \(\beta\)-band, because it has substantial Ce 4f-electron character\(^79\) and the largest DOS at the Fermi energy, namely \(70\%\) of the total DOS.\(^80\) Besides the sizable jump in specific heat, also the remarkable isotropy of \(H_c2\) between the \(ab\)-plane and \(c\)-axis\(^78\) also indicates that the three-dimensional Fermi surface of the \(\beta\)-band is mainly responsible for the superconductivity in CePt\(_3\)Si. In Appendix B we will investigate the other dispersion relation which favors the \(d_{x^2-y^2}\)-wave superconductivity.

As for the AFM order, we assume the staggered field pointing along the [100]-direction \(\vec{h}_Q = hQ\hat{x}\), with \(Q = (0, 0, \pi)\) following the experimental results of CePt\(_3\)Si.\(^57\) For the magnitude we assume \(hQ \ll W\), the band width. This is consistent with the small observed magnetic moment \(\sim 0.16\mu_B\) in CePt\(_3\)Si.\(^57\) The AFM moment is expected to be small also in CeRhSi\(_3\) and CeIrSi\(_3\) since superconductivity occurs near the AFM quantum critical point.

The fourth term \(H_Z\) is the Zeeman coupling term due to the applied magnetic field. We have defined \(\vec{h} = \frac{1}{2} g \mu_B \vec{H}\) where \(g\) is the \(g\)-factor of quasiparticles and \(\mu_B\) is the Bohr magneton. The paramagnetic depairing effect on the superconductivity is characterized by the dimensionless coupling constant \(h/T_c\) with \(h = |\vec{h}|\).

The last term \(H_1\) describes the effective interaction leading to the SC instability and includes three coupling constants, \(U\), \(V\) and \(J\). We assume the on-site interaction \(U\) and the interaction between the nearest neighbor sites in the \(ab\)-plane \(V\). The coupling constant \(J\) describes the part of interaction arising from the AFM order which is anisotropic. According to the random phase approximation (RPA) for the Hubbard model,\(^27\),\(^62\) the SC order parameter is affected by the AFM order mainly through the anisotropy of effective interaction, which can be described by the \(J\)-term in eq. (31).

In the following we examine two parameter sets,

(A) \(U > 0\), \(V = -0.8U\),

(B) \(U < 0\), \(V = 0\). \(\tag{34}\)

The amplitude of \(U\) is chosen so that \(T_c = 0.01\) at zero magnetic field. The ground state is dominantly (A) \(p\)-wave and (B) \(s\)-wave, respectively. Hereafter we simply call these states \(p\)-wave and \(s\)-wave state, respectively. The parameter set (A) is the most important for our purpose, because the \(p\)-wave symmetry is the most promising candidate for the pairing state in CePt\(_3\)Si.\(^\text{21, 27, 29, 85, 86}\)

Although the spin triplet superconductivity is handicapped due to the lack of inversion symmetry in non-centrosymmetric systems according to the Anderson’s theorem,\(^87\) the depairing effect arising from the ASOC vanishes (or is at least smallest) in the \(p\)-wave state.
with \( \vec{d}(\vec{k}) \parallel \vec{g}(\vec{k}) \). This condition is not satisfied in the realistic model, however the depairing effect due to the ASOC is almost avoided in the \( p \)-wave state with \( \vec{d}(\vec{k}) = -p_x \hat{x} + p_y \hat{y} \). Another parameter set (B) is investigated as a typical model for the dominantly spin singlet pairing state. We will investigate the dominantly \( d_{z^2 - r^2} \)-wave state in Appendix B and obtain qualitatively the same results as the \( s \)-wave state.

Before analyzing the effective model in eq. (29), we comment on the RPA theory applied to the Hubbard model for the \( \beta \)-band of CePt\(_3\)Si. This theory leads to two possible pairing states due to spin fluctuation mediated interaction: the \( s + P \)-wave and the \( p + D + f \)-wave state. The former is dominated by the \( p \)-wave component and can be viewed as an intra-plane pairing state, while the latter is described by the inter-plane pairing dominated by the \( d_{xz} \) and \( d_{yz} \)-wave components. Here we focus on the \( s + P \)-wave state whose order parameter is reproduced by assuming the parameter set (A) and \( J = 0.3V \) \((J = 0)\) for \( h_Q = 0.125 \) \((h_Q = 0)\) in eq. (29).

On the other hand, the \( p + D + f \)-wave state is not realized in eq. (29) because the inter-plane interaction is neglected. It is expected that the paramagnetic properties in the inter-plane \( d \)-wave state are qualitatively the same as those in the intra-plane \( s \)- and \( d \)-wave states. The other characteristic properties of the \( p + D + f \)-wave state will be discussed in §6 and §7.

To solve the effective model eq. (29), we apply the mean field theory and obtain the mean field equations as,

\[
\Delta_{i,s,s'}(\vec{k}) = -T \sum_{n,\vec{k}'} \mathcal{U} \left\{ V + \left( \frac{J}{2} C(\vec{k} - \vec{k}') \right) \right\} \times F_{i,s,s'}(\vec{k}', \omega_n), \tag{35}
\]

\[
\Delta_{i,s,s'}(\vec{k}) = -T \sum_{n,\vec{k}'} C(\vec{k} - \vec{k}') \{ VF_{i,s,s'}(\vec{k}', \omega_n) \}
\]

\[ -\frac{J}{2} F_{i,s,s'}(\vec{k}', \omega_n) \]. \tag{36}

The normal and anomalous Green functions \( G_{i,s,s'}(\vec{k}, \omega_n) \), \( F_{i,s,s'}(\vec{k}, \omega_n) \) in the spin basis are obtained by the Dyson-Gorkov equation,

\[
\begin{pmatrix}
\hat{G}_N(\vec{k}, \omega_n)^{-1} & \hat{\Delta}_{\text{spin}}(\vec{k}) \\
\hat{\Delta}_{\text{spin}}(\vec{k})^\dagger & -\hat{G}_N(\vec{k})^{-1}
\end{pmatrix}
\times
\begin{pmatrix}
\hat{G}(\vec{k}, \omega_n) \\
\hat{\tilde{F}}(\vec{k}, \omega_n)
\end{pmatrix}
= \hat{1}. \tag{37}
\]

where \( \hat{X}(\vec{k}) \) \((X = G, F, \Delta_{\text{spin}})\) is the \( 4 \times 4 \) matrix,

\[
\hat{X}(\vec{k}) = \begin{pmatrix}
X_{1,ss'}(\vec{k}) & X_{2,ss'}(\vec{k}) \\
X_{2,ss'}(\vec{k} + \vec{Q}) & X_{1,ss'}(\vec{k} + \vec{Q})
\end{pmatrix}. \tag{38}
\]

The normal Green function in the normal state, \( \hat{G}_N(\vec{k}, \omega_n) \) is obtained as \( \hat{G}_N(\vec{k}, \omega_n) = (i\omega_n \hat{1} - \hat{H}(\vec{k}))^{-1} \) by using eq. (8) with \( \tilde{h}_Q = h_Q \hat{x} \) and \( \hat{e}(\vec{k}) = \epsilon(\vec{k}) \hat{\delta}^{(0)} + \alpha \hat{g}(\vec{k}) \cdot \hat{\delta} \).

We here discuss the symmetry of the SC state on the basis of the following parameterization of order parameters:

\[
\Delta_{1,s,s'}(\vec{k}) = \begin{pmatrix}
-d_x(\vec{k}) + id_y(\vec{k}) & \Phi(\vec{k}) + d_z(\vec{k}) \\
-\Phi(\vec{k}) + d_z(\vec{k}) & d_x(\vec{k}) + id_y(\vec{k})
\end{pmatrix}, \tag{39}
\]

where we use the even parity scalar function \( \Phi(\vec{k}) \) and the odd parity vector \( \vec{d}(\vec{k}) \). Although a second component \( \Delta_{s,s'}(\vec{k}) \) appears in the AFM state, the basic properties and symmetries are little affected by \( \Delta_{s,s'}(\vec{k}) \).

| P-wave state | Even parity part | Odd parity part |
|--------------|-----------------|----------------|
| PM at \( \vec{h} = 0 \) | \( \kappa(\delta + c_x + c_y) \) | \( -\eta_y s_x, 0 \) |
| AFM at \( \vec{h} = 0 \) | \( \kappa(\delta + c_x + c_y) \) | \( -\eta_y s_x, 0 \) |
| AFM at \( \vec{h} = h \tilde{y} \) | \( \kappa(\delta + c_x + c_y) \) | \( -\eta_y s_x, 0 \) |

Table 1. Symmetry of order parameter in the dominantly \( p \)-wave state. We use the abbreviations \( c_{x,y} = \cos k_{x,y} \) and \( s_{x,y} = \sin k_{x,y} \). We assume the PM state at zero magnetic field, the AFM state at zero magnetic field and the AFM state under the magnetic field \( \vec{h} \parallel \hat{y} \) from the top to the bottom. The parameters \( \beta, \gamma, \kappa, \delta \) and \( \eta \) are real.

In Table I we summarize the order parameters in the \( p \)-wave state. The admixture with the even-parity component due to the ASOC is expressed by the parameter \( \kappa \) which is in the order of \( \alpha/eF \). We obtain \( \kappa \sim 0.15 \) for \( \alpha = 0.3 \). The even-parity part \( \Phi(\vec{k}) \) is dominated by the extended \( s \)-wave component and \( \delta \sim 0.2 \) because the conventional \( s \)-wave component is suppressed by the strong on-site repulsion \( U \). The \( d_{xz} \)-component of the odd parity vector \( \vec{d}(\vec{k}) \) is induced by the magnetic field \( \gamma \propto h/\sqrt{2} \) to gain the Zeeman energy. The SC state is mainly affected by the parameter \( \beta \) which is unity in the absence of AFM order and magnetic field. The magnetic field along the \([010]-axis \) \([100]-axis \) decreases \( (increases) \) \( \beta \). The influence of the AFM order depends on the value of \( J \). We find \( \beta \sim 0.3 \) \(( \beta \sim 3.7) \) for \( J = 0.3V \) \((J = 0) \) at \( h_Q = 0.125 \) and \( h = 0 \). The deviation from \( \beta = 1 \) can be viewed as the mixing between \( \vec{d}(\vec{k}) \sim (\sin k_x, \sin k_z, 0) \) and another \( p \)-wave state \( \vec{d}(\vec{k}) \sim (\sin k_x, \sin k_z, 0) \). Although these pairing states belong to different irreducible representations of the \( D_{4b} \) symmetry, they are mixed due to the presence of the symmetry reducing AFM moment or magnetic field.

In general, the dominantly \( s \)-wave state is admixed to the \( p \)-wave state due to the ASOC and belongs to the same irreducible representation as the dominantly \( p \)-wave state realized for the parameter set (A). However, only the conventional \( s \)-wave component \( \Phi(\vec{k}) = 1 \) appears and \( \vec{d}(\vec{k}) = \vec{0} \) for the parameter set (B) because only the on-site interaction is taken into account \((V = J = 0) \). Generally speaking, the admixture of spin singlet and triplet order parameters plays no important role when the ASOC is much smaller than the Fermi energy, \( |\alpha| \ll eF \).

The "helicity" \( \vec{q}_{11} \)-vector is perpendicular to the magnetic field as will be discussed in §8 in details. The amplitude of \( \vec{q}_{11} \) below \( T_c \) should be determined to maximize the condensation energy. However, we here determine \( \vec{q}_{11} \) at \( T = T_c(h) \) and neglect the temperature dependence.
below $T_c$ for simplicity. The transition temperature $T_c(h)$ is determined by linearizing the mean field equation as,

$$\lambda(\vec{q})\Delta_{i,s,s}(\vec{k}) = -T \sum_{n,k'} (U + (V - \frac{J}{2})C(\vec{k} - \vec{k}')) \times \phi_{i,s,s}(\vec{k}',\omega_n),$$

$$\lambda(\vec{q})\Delta_{i,s,s}(\vec{k}) = -T \sum_{n,k'} C(\vec{k} - \vec{k}') \times \{V \phi_{i,s,s}(\vec{k}',\omega_n) - \frac{J}{2} \phi_{i,s,s}(\vec{k}',\omega_n)\},$$

where $\phi_{i,s,s}(\vec{k}',\omega_n)$ is obtained by linearizing the anomalous Green function $F_{i,s,s}(\vec{k}',\omega_n)$ with respect to $\Delta_{\text{spin}}(\vec{k})$. We optimize the eigenvalue $\lambda(\vec{q})$ with respect to the order parameter $\Delta_{\text{spin}}(\vec{k})$ and the helicity $\vec{q} = \vec{q}_H$. The transition temperature $T_c(h)$ is determined by the criterion $\lambda(\vec{q}_H) = 1$.

We have estimated the condensation energy below $T_c$ and found that the magnitude of $\vec{q}_H$ increases as decreasing the temperature. However, we have confirmed that the temperature dependence of $\vec{q}_H$ can be ignored for the magnetic properties discussed in the following part.

4. $s$-wave State

For the discussion of non-linear response to the magnetic field in NCSC we first discuss the simplest case, namely the $s$-wave state without AFM order. We address the enhancement of the critical magnetic field $h_{c2} = \frac{1}{2}g\mu_B H_{c2}$ due to the ASOC, assuming the parameter set (B) $U < 0$ and $V = 0$. Figure 2 shows the phase diagram, temperature $T/T_c$ versus magnetic field $h/T_c$ along the [100]- or [010]-direction. The critical field $h_{c2}$ for both the uniform state ($\vec{q}_H = 0$) and the helical state ($\vec{q}_H \neq 0$) are depicted, whereby also the behavior in the absence of ASOC ($\alpha = 0$) is included for a comparison.

As we focus here on the paramagnetic limiting effect, we neglect the orbital depairing for simplicity. Note that $h_{c2}$ in the helical $s$-wave state has been investigated in Ref. 35 for an isotropic Fermi surface.

The data in Fig. 2 demonstrate that the $h_{c2}$ is significantly enhanced by the ASOC. This is partly due to the residual spin susceptibility in the SC state induced by the ASOC. Neglecting the magnetic field dependence of the spin susceptibility, we obtain a simple estimation for the critical magnetic field,

$$h_{c2} = \sqrt{\frac{2E_c}{\chi^S - \chi^N}}.$$

where $E_c$ is the condensation energy and $\chi^S$ and $\chi^N$ are the spin susceptibility in the SC and normal state, respectively. According to eq. (42), $h_{c2}$ increases by a factor of $\sqrt{2}$ because of the residual spin susceptibility $\chi^S = \frac{1}{2}\chi^N$ at $T = 0$. In fact, $h_{c2}$ is enhanced even more due to the magnetic field dependence of spin susceptibility. A further enhancement of $h_{c2}$ is caused by the formation of a helical SC state, which exceeds the enhancement in centrosymmetric superconductor owing to the presence of an FFLO state.88

![Fig. 2. (Color online) The $H$-$T$ phase diagram in the $s$-wave state for the magnetic field along the [100]- or [010]-axis. The diamonds (circles) show the reduced critical magnetic field $h_{c2}/T_c = \frac{1}{2}g\mu_B H_{c2}/T_c$ in the helical (uniform) SC state against the reduced temperature $T/T_c$. We assume $U < 0$, $V = 0$, $J = 0$, $\alpha = 0.3$ and $\hbar_Q = 0$. The phase diagrams in the absence of ASOC ($\alpha = 0$) are shown for a comparison. The dashed and solid lines show the $h_{c2}/T_c$ in the uniform ($\vec{q}_H = 0$) and FFLO ($\vec{q}_H \neq 0$) states, respectively.](image)

![Fig. 3. (Color online) The $H$-$T$ phase diagram in the helical $s$-wave state with AFM order. We assume $\hbar_Q = 0.125\xi$. The other parameters are the same as Fig. 2. The circles and triangles show the $h_{c2}$ for the magnetic field along the [010] and [100]-axis, respectively. The $h_{c2}$ in the PM state is shown for a comparison (diamonds).](image)
5. The $p$-wave State

We here investigate the dominantly $p$-wave state which is the most promising candidate for the pairing state in CePt$_3$Si. In this section we assume the parameter set ($\Delta$) $U > 0$, $V = -0.8U$.

5.1 PM state

To illuminate the difference with the dominantly spin singlet pairing state we again turn to the PM state. We find that paramagnetic depairing effect is naturally less effective in suppressing the onset of superconductivity. Figure 4 shows $h_{c2}$ for the $p$-wave state which is much higher than for the case of $s$-wave as well as $d$-wave pairings. This is rather surprising because the $h_{c2}$ is independent of the pairing symmetry considering only the simple estimation in eq. (42). Actually, $h_{c2}$ of the $p$-wave state is enhanced by the modification of SC order parameters due to the mixing with $\vec{d}(\vec{k}) = (\sin k_y, \sin k_x, 0)$ in addition to the formation of helical SC state. Since the $p$-wave superconductivity has a multi-component order parameter with respect to the spin, the order parameter can be modified to optimally cope with the competition between the Zeeman coupling energy and ASOC. This is not the case in the dominantly spin singlet pairing state. This is the main reason why the paramagnetic depairing effect in NCSC depends on the symmetry of the leading order parameter. We see that the $h_{c2}$ curves in Fig. 4 merge in the low magnetic field region where the linear response theory is justified.

In order to shed light on the mechanisms stabilizing the $p$-wave superconductivity at high magnetic fields, i.e., (i) the formation of helical SC state, and (ii) the modification of SC order parameters, we compare $h_{c2}$ with the one for the uniform state with $\vec{q}_H = 0$ (triangles in Fig. 5) and the one for the SC state with $\vec{d}(\vec{k}) = (-\sin k_y, \sin k_x, 0)$, $\Phi(\vec{k}) = 0$ and $\vec{q}_H = 0$ (diamonds in Fig. 5). Both (i) and (ii) are neglected in the latter (diamonds) while (i) is neglected in the former (triangles). The comparison between the triangles and diamonds shows the enhancement of $h_{c2}$ by optimizing the SC order parameter. Actually, the $a_x$-($d_x$-)component of $d$-vector decreases in the magnetic field along the [100]-([010]-)axis to avoid the paramagnetic depairing effect. The $h_{c2}$ is furthermore enhanced below $T = 0.6T_c$ by forming the helical SC state (circles). Thus, the $p$-wave superconductivity can be stabilized in the magnetic field which is much higher than the standard paramagnetic limit owing to the combination of mechanisms (i) and (ii).

A large critical magnetic field $h_{c2}$ generally indicates that a SC state with a large spin susceptibility is stabilized at high magnetic fields. The general spin susceptibility defined by $\chi_a = \chi_b = M_{x,y} / h$ is obtained from the calculation of the uniform magnetization,

$$M_\mu = \sum_k \text{Tr} S^\mu \hat{G}(k),$$

(43)
5.2 Role of anisotropic Fermi surface

A further important role in this context is played by the shape of the Fermi surface. The band structure of the $\beta$-band is complicated but has one eye-catching property: the cross sections of the Fermi surface in the range $k_x > 2\pi/3$ are quadrilateral with the corners along the [110]- and [1-10]-directions.\cite{27,80} We show the schematic figures for the Fermi surface in Fig. 7 where the anisotropy is stressed for simplicity. The anisotropy of the Fermi surface affects $h_{c2}$ in two ways, by facilitating (i) the formation of the helical SC phase and (ii) the modification of the SC order parameters, as we will discuss now.

First, (i) the helical SC phase is stable for the anisotropic Fermi surface not only in the $p$-wave state but also in the $s$- and $d$-wave states. This is simply because a set of quasi-particles with $\vec{k} = \pm \vec{k} + \vec{q}_H/2$ can have low energy on a large part of the first Brillouin zone (nesting feature of the Fermi surface). As shown in Fig. 7(b), the large (small) Fermi surface moves to the right (left) in the magnetic field along the [010]-axis. Under this condition, uniform Cooper pairing on the Fermi surface part parallel to [010]-axis (part “II” in Fig. 7(b)) is destabilized, while it is little affected on the part “I”. However, the depairing effect arising from the large Fermi surface is essentially avoided in the helical SC phase having $\vec{q}_H \sim 2\hbar/\sqrt{\pi}x$ (Fig. 7(c)) because of the nesting of Fermi surface along the [100]-direction. This leads to the strong enhancement of $h_{c2}$. This is not the case in the isotropic system where the Fermi surface is not nested.

Second, the anisotropic Fermi surface enhances (ii) the mixing of order parameters and increases in this way $h_{c2}$ in the $p$-wave state. Because of the structure of $g$-vector $g(\vec{k}) \propto (-v_x(\vec{k}), v_y(\vec{k}), 0)$, the SC gap on the Fermi surface perpendicular to the [010]-axis (Fermi surface “$I$” in Fig. 7(b)) is mainly induced by the $d_\alpha$-component of spin triplet order parameter while the $d_\beta$-component is the main source of the SC gap on the other part (Fermi surface “$II$” in Fig. 7(b)). Since the $d_\alpha$- and $d_\beta$-components induce the Cooper pairing on different parts of the Fermi surface, the coupling is weak between these two order parameters. Hence, the splitting of energy between $d(\vec{k}) = (-\sin k_x, \sin k_y, 0)$ (most stable state) and $d(\vec{k}) = (\sin k_x, \sin k_y, 0)$ (second most stable state) due to the ASOC is small, and they can be easily mixed by the applied magnetic field.

In general, the tetragonal anisotropy of the Fermi surface reduces the splitting between the most stable and the second most stable pairing states. For an isotropic Fermi surface, the second most stable pairing state has 2-fold degeneracy; $\vec{d}(\vec{k}) = (k_x, k_y, 0)$ is degenerate with $\vec{d}(\vec{k}) = (-k_x, k_y, 0)$. However, this degeneracy is lifted by the tetragonal anisotropy as shown in the

\begin{figure}[h]
\centering
\includegraphics[width=0.8\textwidth]{Fig7}
\caption{(Color online) The schematic figure for the Fermi surface and SC gap in the p-wave state. We show the cross section for a fixed $k_x$. Two solid lines show the Fermi surfaces which are split by the ASOC. The dashed lines show the magnitude of SC gap on each Fermi surface. (a) The uniform BCS state at $\vec{H} = 0$. The direction of $d$-vector is shown by the arrows. (b) The uniform BCS state for $\vec{H}//[010]$. The parts of Fermi surface “$I$” and “$II$” are shown. The SC gap on the part “$I$” is suppressed. (c) The helical SC state for $\vec{H}//[010]$. The SC gap on the part “$II$” of large Fermi surface is increased. (d) The helical SC state for $\vec{H}//[110]$.}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=0.8\textwidth]{Fig8}
\caption{(Color online) The schematic figure for the energy levels in the dominantly p-wave state. The isotropic and tetragonal symmetries are assumed in the left and right figures, respectively. The 2-fold degeneracy in the isotropic system between $d(\vec{k}) = (k_x, k_y, 0)$ and $d(\vec{k}) = (-k_x, k_y, 0)$ is lifted to $d(\vec{k}) = (\sin k_y, \sin k_x, 0)$ and $d(\vec{k}) = (-\sin k_x, \sin k_y, 0)$ in the tetragonal system. In case of the $\beta$-band of CePt$_3$Si, $d(\vec{k}) = (\sin k_y, \sin k_x, 0)$ has lower energy.}
\end{figure}
schematic figure (Fig. 8). This lift of degeneracy decreases the difference of condensation energy between $\tilde{d}(\vec{k}) = (-\sin k_y, \sin k_x, 0)$ and $\tilde{d}(\vec{k}) = (\sin k_y, \sin k_x, 0)$ (or $\tilde{d}(\vec{k}) = (-\sin k_y, \sin k_x, 0)$) in the system with tetragonal symmetry (see Fig. 8).

Furthermore, a strong anisotropy of the Fermi surface induces a pronounced 4-fold anisotropy in the paramagnetic properties. Figure 9 shows that the $h_{c2}$ along the [110]-direction is much smaller than that along the [100]-direction in case of the $p$-wave state. This is mainly because the state $\tilde{d}(\vec{k}) = (-\sin k_y, \sin k_x, 0)$ is admixed by the magnetic field along the [110]-direction, with $\tilde{d}(\vec{k}) = (-\sin k_x, \sin k_y, 0)$, but not with $\tilde{d}(\vec{k}) = (\sin k_x, \sin k_y, 0)$. The latter is less stable than the former in case of the $\beta$-band of CePt$_3$Si. On the other hand, the 4-fold anisotropy is weak for the $s$-wave state as shown by the squares in Fig. 9. This indicates that the anisotropic Fermi surface enhances the $h_{c2}$ in the $p$-wave state mainly through the mixing of SC order parameters.

Finally, we comment on orbital depairing which we have neglected so far. The orbital depairing effect is reduced by the mixing of order parameters in the $p$-wave state. For example, the parameter $\beta$ in $\tilde{d}(\vec{k}) = (-\sin k_y, \beta \sin k_x, -i\gamma \sin k_y)$ is decreased by the magnetic field along the [010]-direction, and reduces the orbital depairing effect, because the coherence length along the [100]-direction shrinks. Thus, the $h_{c2}$ in the $p$-wave state is enhanced by modifying the order parameter through the suppression of the orbital depairing effect as well as the paramagnetic depairing effect.

5.3 AFM state

In the discussion of the influence of AFM order on the $p$-wave SC state we focus on staggered moments along the [100]-axis with the magnetic field parallel to the [010]-axis, since the AFM moment favors to be perpendicular to the field. The situation of the magnetic field parallel to the moment is described in §7.

The influence of the AFM order on the $p$-wave state significantly depends on the anisotropic spin-spin interaction, the $J$-term in eq. (31). The critical field $h_{c2}$ depicted in Fig. 10 with $h_Q = 0.125$ in the AFM ordered phase shows a clear trend. While the AFM leads to a reduction of $h_{c2}$ in the absence of the anisotropic spin interaction ($J = 0$), a strong enhancement is obtained for $J = 0.3$.

We understand these results by analyzing the parameter $\beta$ of $\tilde{d}(\vec{k}) = (-\sin k_y, \beta \sin k_x, 0)$ at zero magnetic field.

For $\beta < 1$, the superconductivity is dominant on Fermi surface region “I” in Fig. 7(b), while the magnetic field along the [010]-axis suppresses Cooper pairing on the Fermi surface “II”. For this reason, this SC state is robust against the magnetic field along the [010]-axis. The magnetic field reduces $\beta$ even more enhancing the anisotropy of the SC gap. The enhancement of $h_{c2}$ due to the AFM order is much more significant than expected in the simple estimation eq. (42). In fact, the suppression of paramagnetic depairing effect in case of $\beta < 1$ can be viewed as a result of the strong non-linear response to the magnetic field. The small energy scale $\beta T_c$ appears in this case and induces the strong non-linearity. This is the reason why the influence of AFM order is much more important in the $p$-wave state than in the $s$-wave state. If we assume $J = 0$, the parameter $\beta$ is more than unity, which is incompatible with our RPA analysis for the Hubbard model. On the other hand, we obtain $\beta \sim 0.3$ for $J = 0.3V$ and $h_Q = 0.125$, giving the result consistent with the RPA theory.

The strong non-linear response to the magnetic field clearly appears in the magnetic field dependence of spin susceptibility. We show the spin susceptibility $\chi_b$ for $J = 0.3V$ ($\beta < 1$) and $J = 0$ ($\beta > 1$) in Figs. 11 (a) and (b), respectively. For low magnetic fields ($h = 0.1 T_c$) $\chi_b$ is enhanced by AFM order in both cases consistent with the linear response theory (§2.4). We find that $\chi_b$ is furthermore enhanced for the moderate magnetic field $h = T_c$ with $\beta < 1$ (Fig. 11(a)) although the critical temperature $T_c(h)$ is little decreased. According to these
For the high critical field $H_c$ have been shown in Figs. 10 and 11(a). These findings could be understood based on the $\mu$SR measurement by Yogi et al. $^{27,30,31,63-65}$ and the line node behaviors in various quantities. Moreover the microscopic theory within an RPA theory suggests an in-plane $p$-wave state induced by the $\beta$-band of CePt$_3$Si. $^{27}$

For $\vec{H} \perp \vec{h}_Q$, the experimental magnetic properties of CePt$_3$Si at ambient pressure are consistent with the $p$-wave state with $\beta < 1$. This indicates the strong anisotropy of the effective spin interaction, which is described by the $J$-term in eq. (31) and is compatible with the RPA analysis. $^{27}$ It does however not agree with the naive second order perturbation theory which leads to the $p$-wave state with $\beta > 1$. $^{62}$ This is because the role of spin fluctuation is underestimated within the perturbation theory. $^{93}$ Based on this fact we may state that there is some evidence for spin-fluctuation-mediated superconductivity in CePt$_3$Si.

When the magnetic field is parallel to the AFM moment $\vec{H} \parallel \vec{h}_Q$, the paramagnetic depairing effect is enhanced (suppressed) in the $p$-wave state with $\beta < 1$ ($\beta > 1$). We have confirmed that the $h_{c2}$ for $\vec{H} \parallel \vec{h}_Q$ with $\beta > 1$ is qualitatively the same as the $h_{c2}$ for $\vec{H} \perp \vec{h}_Q$ with $\beta < 1$ (squares in Fig. 10). If the sample had a domain structure with respect to the direction of AFM moment, the SC state with the maximal $T_c$ would mark the SC transition. Under such circumstances $p$-wave states with both $\beta > 1$ and $\beta < 1$ could “avoid” the paramagnetic depairing effect and would be consistent with the experimental results in CePt$_3$Si. $^{1,2,7,58,66,67}$

We here comment on the inter-plane $d$-wave state which we found as another possible pairing state on the basis of the RPA theory. $^{27}$ Although the 2-fold degeneracy exists in this state ($d_{xz,z}$- and $d_{yz}$-wave), the order parameter has no internal degree of freedom with respect to the spin. Therefore, the paramagnetic depairing effect cannot be avoided by modifying the order parameter in contrast to the $p$-wave state. Hence, the magnetic properties are qualitatively the same as those in the $s$-wave state which seem to be incompatible with the experimental results in CePt$_3$Si. The inter-plane $d$-wave state is incompatible with the coherence peak in the NMR $1/T_1T$ too. $^{92}$

7. Proposals for test experiments

Here we discuss several experiments which could help to establish the pairing symmetry for CePt$_3$Si as well as CeRhSi$_3$ and CeIrSi$_3$.

The influence of antiferromagnetism on the magnetic properties can be tested by using the fact that AFM theoretical results, the NMR Knight shift measurement $^{66}$ by Yogi et al. and the $\mu$SR measurement $^{67}$ by Higemoto et al. were carried out in the non-linear response regime. In contrast to $\beta < 1$, the moderate magnetic field $h = T_c$ little affects the spin susceptibility (Fig. 11(b)). The non-linearity of spin susceptibility appears only in the high field region close to the critical magnetic field. This is a characteristic property of the SC state with strong paramagnetic depairing effect such as the spin singlet pairing state in centrosymmetric system. Qualitatively the same magnetic field dependence is obtained in the dominantly $d_{x^2-y^2}$-$\pm$-wave state (see Fig. B.1 in Appendix B).

6. Pairing symmetry in CePt$_3$Si

Measurements of $H_{c2}$ and the Knight shift are consistent with $p$-wave superconductivity in CePt$_3$Si at ambient pressure. The temperature dependence of $H_{c2}$ $^{1,2,7,58}$ implies the absence of paramagnetic depairing. NMR and $\mu$SR Knight shift data show no decrease below $T_c$ $^{66,67}$ although $T_c$ remains rather high at applied magnetic fields. These findings could be understood based on the $p$-wave state with AFM order for which the theoretical results have been shown in Figs. 10 and 11(a).

We here note that the other possible mechanisms for the high critical field $H_{c2}$ are unlikely relevant in CePt$_3$Si. For example, a small $g$-factor has been suggested for CeCoIn$_5$ ($g \sim 0.63$). $^{89}$ It is expected that the $g$-factor of CeCoIn$_5$ is significantly renormalized by the strong AFM correlation in the $ab$-plane. $^{90}$ However, this is not the case in CePt$_3$Si where the spin correlation in the $ab$-plane are dominantly ferromagnetic. $^{27,57}$ The strong coupling effect which has been ignored in this paper is another possible cause of high $H_{c2}$. But, the jump of the specific heat at $T = T_c$ does not indicate strong coupling effects in CePt$_3$Si. $^{1,2,7,65}$ in contrast to CeIrSi$_3$. $^{91}$

Fig. 11. (Color online) The spin susceptibility along the [010]-direction in the helical $p$-wave state with AFM order. We assume $J = 0.3'V$ leading to $\beta < 1$ in (a) and $J = 0$ leading to $\beta > 1$ in (b), respectively. The magnetic field is shown in the figures. The other parameters are the same as in Fig. 10.
order can be suppressed by pressure in these materials.\(^4\)-7,59,60 It follows from our results in §4, §5.1 and Appendix B, that in the purely SC phase the paramagnetic depairing should limit the upper critical field for \(\vec{H} \parallel ab\) and the spin susceptibility should decrease below \(T_c\) in the low-magnetic field regime. Actually recent measurements of \(H_{c2}\) along \(ab\)-plane in CeRhSi\(_3\)\(^5\),\(^7\) and CeIrSi\(_3\)\(^7\),\(^6\),\(^8\),\(^78\) imply a clear paramagnetic depairing effect in the purely SC region, consistent with the theoretical view. Notably paramagnetic depairing seems less effective in the AFM state of CeIrSi\(_3\)\(^7\). This is compatible with \(p\)-wave pairing. No studies of this kind have been performed so far for CePt\(_3\)Si.

A further aspect is the 2-fold in-plane anisotropy in the AFM state. Since the \([100]\) - and \([010]\)-axes are not equivalent in the AFM state, a 2-fold anisotropy appears in the \(ab\)-plane. Although the AFM moment perpendicular to the uniform magnetic field is generally favored, the situation \(\vec{H} \parallel \vec{h}_Q\) can nevertheless be realized for magnetic fields low enough to leave the orientation of the AFM moment unchanged.

We summarize the 2-fold anisotropy expected for each pairing state in Fig. 12 taking also the orbital depairing effect into account. We assumed here that the \(H_{c2}\) determined by the orbital depairing is much higher than the standard paramagnetic limit field in CePt\(_3\)Si\(^1\),\(^2\)\(^7\),\(^5\)\(^8\) CeRhSi\(_3\)\(^4\),\(^5\) and CeIrSi\(_3\)\(^7\),\(^6\)\(^8\) The upper critical field due to orbital depairing is naturally enhanced by the heavy mass of quasi-particles in these heavy Fermion compounds. Under such conditions paramagnetic depairing can play a role in the high-field regime. Fig. 12(a) shows the \(H-T\) phase diagram in the \(p\)-wave state. For \(\vec{H} \parallel \vec{h}_Q\) the paramagnetic depairing effect is enhanced (suppressed) with \(\beta < 1\) (\(\beta > 1\)). Note that the opposite occurs for \(\vec{H} \perp \vec{h}_Q\) (see Fig. 10). Therefore, a significant 2-fold anisotropy of \(H_{c2}\) could appear at high magnetic fields for either \(\beta < 1\) or \(\beta > 1\), provided the AFM moment remains pinned. Qualitatively the same anisotropy would occur at low magnetic fields, because the orbital depairing effect is anisotropic owing to the in-plane anisotropy of coherence length, namely the difference of \(\xi_a\) and \(\xi_b\). On the basis of the RPA theory for CePt\(_3\)Si\(^2\) we have estimated the anisotropy as \(\partial H_{c2}/\partial T\big|_{T = T_c}(\vec{H} \parallel [100]) : \partial H_{c2}/\partial T\big|_{T = T_c}(\vec{H} \parallel [010]) = \xi_a : \xi_b = 0.672 : 1\) at \(h_Q = 0.125\). Thus, the \(H-T\) phase diagram is highly anisotropic in both high and low magnetic field region as shown in Fig. 12(a).

The strong 2-fold anisotropy in the \(ab\)-plane appears also in the inter-plane \(d\)-wave state due to the anisotropy of the coherence length. The 2-fold degeneracy between the \(d_{xz}\) - and \(d_{yz}\)-wave states is lifted by the AFM order. The staggered moment along the \([100]\)-axis favors the \(d_{xy}\)-wave state and yields a coherence length which is longer along the \([100]\)-axis than along the \([010]\)-axis. For this reason \(H_{c2}\) close to \(T = T_c\) is smaller for the magnetic field along the \([010]\)-axis. This anisotropy is suppressed at high magnetic fields because the paramagnetic depairing effect is nearly isotropic in the \(s\)-wave state (Fig. 3). These considerations lead to the schematic phase diagram in Fig. 12(b).

It should be noted that the in-plane anisotropy of \(H_{c2}\) in the inter-plane \(d\)-wave state does not vanish if the quantum critical point of the AFM order is approached. This is in contrast to the \(p\)-wave state where the in-plane anisotropy is suppressed by decreasing the AFM moment. In the vicinity of AFM quantum critical point, multiple phase transitions can occur for the inter-plane \(d\)-wave state as discussed in Ref. 27. These multiple phases in the \(H-T\) plane are shown in Fig. 12(c) for the magnetic field along the \([010]\)-axis. Pure \(d_{xz}\)- and \(d_{yz}\)-wave states appear in the high-temperature region and in the high-magnetic field region, respectively. The chiral \(d_{xz} \pm id_{yz}\)-wave state is stabilized at low temperatures and fields. If the multiple phase transitions were observed in the \(H-T\) plane or in the \(P-T\) plane, it would be a strong evidence for the inter-plane \(d\)-wave state. Although some indications for a second SC transition have been reported in CePt\(_3\)Si\(^6\)\(^4\),\(^9\)-\(^6\) it remains unclear whether it represents an intrinsic property or is caused by the sample inhomogeneity.

In contrast to the \(p\)-wave and inter-plane \(d\)-wave states, the 2-fold anisotropy of \(H_{c2}\) is very weak in the intra-plane \(d\)-wave and \(s\)-wave states because the paramagnetic depairing effect as well as the orbital depairing effect are nearly isotropic. Therefore, we obtain a simple phase diagram in Fig. 12(d).

Since the 2-fold anisotropy of \(H_{c2}\) is quite different between the dominantly \(p\)-wave, inter-plane \(d\)-wave and intra-plane spin singlet pairing states, the future experiment in the AFM state could identify the pairing symmetry in CePt\(_3\)Si, CeRhSi\(_3\) and CeIrSi\(_3\). It should be noticed that this experiment can be performed in CePt\(_3\)Si without applying the pressure.
8. Helical Superconductivity

In this section we discuss the nature of the helical SC state which is a novel SC phase specific to NCSC. The SC phase with a finite total momentum of Cooper pairs $\vec{q}_H$ is stabilized in the presence of Rashba-type spin-orbit coupling under a magnetic field in the $ab$-plane. This state bears some similarity with the FFLO state in centrosymmetric superconductors, but has important differences. First, the helical SC phase is stabilized immediately above $H_c2$ which is much lower than $H_c2$ in the type II superconductors. This is in contrast to the FFLO state which appears in a narrow region near $H_c2$ only. Second, the phase of SC order parameter is modulated as $\Delta(\vec{r}) = \Delta e^{i\vec{q}_H \cdot \vec{r}}$ in the helical SC state (which is the same form as in the Fulde-Ferrell (FF) state) while the Larkin-Ovchinnikov (LO) state with the spatial modulation of the amplitude, $\Delta(\vec{r}) = \Delta \cos \vec{q}_H \cdot \vec{r} = \Delta (e^{i\vec{q}_H \cdot \vec{r}} + e^{-i\vec{q}_H \cdot \vec{r}})/2$, is more stable than the FF state.97

Because the two momenta $\vec{q}_H$ and $-\vec{q}_H$ are equivalent in the centrosymmetric system, the order parameter has a double $q$ structure in the LO state. On the other hand, $\vec{q}_H$ is not equivalent to $-\vec{q}_H$ in the non-centrosymmetric system under a magnetic field. For this reason the helical SC phase is realized in the NCSC at least just below the critical temperature. At higher fields and low temperatures also a “stripe SC state” can be realized which is similar to the LO state.

Experimental evidence for the FFLO state has been obtained for CeCoIn$_5$ more than forty years after the theoretical proposal.98 This is because the FFLO state is suppressed by a weak disorder.99 The stripe SC state, which resembles the FFLO state, can be suppressed by a weak disorder too. In contrast to these states the helical SC state is realized even in the disordered material, if the superconductivity is present. Although there is no experimental verification of the helical SC state in NCSC so far, the existence of the helical SC phase is a mandatory feature from a theoretical point of view.

Now we turn to the effect of finite $\vec{q}_H$ on the paramagnetic properties. Although the influence of the helical superconductivity has been taken into account in §§4 and 5, the following discussion will be important for a deeper understanding.

One of the characteristic properties in the helical SC state is the presence of a finite spin magnetization. In the low magnetic field region this magnetization is expressed as $\vec{M} = \vec{M}_0 + \chi \vec{H}$ with finite $\vec{M}_0$. For simplicity, we here consider the PM state and assume the SC order parameter without gap nodes. Then, the magnetization is obtained as,

$$\vec{M}_0 = \frac{1}{4} \sum \vec{g}(\vec{k})(\vec{B}_1(\vec{k}) \cdot \vec{q}_H - \vec{B}_2(\vec{k}) \cdot \vec{q}_H)$$

$$\approx \frac{1}{2} \int d\vec{k} F(\vec{k})/v_1(\vec{k})/v_1(\vec{k}) - (1 \leftrightarrow 2)$$

$$= D (\hat{z} \times \vec{q}_H),$$

with $D \propto \alpha$. We define $\vec{B}_i(\vec{k}) = d(c_\gamma(\vec{k})/E(\vec{k}))d\vec{k}$ where $\gamma$ is a band index. As shown in eq. (46), the magnetization is oriented along the direction perpendicular to $\vec{q}_H$. The helical superconductivity also affects the differential spin susceptibility $\chi_{\mu\nu} = dM_\mu/dH_\mu$ when the SC gap has a node. According to eqs. (11-13), the quasi-particles suffer a Doppler shift in the helical SC state and the single particle excitation energy is expressed as $\sqrt{\epsilon(\vec{k})^2 + |\Delta(\vec{k})|^2}$. Following eq. (15), the Pauli part of differential spin susceptibility is obtained as,

$$\chi^P_{\mu\nu} = \sum_\gamma d\vec{k} F(\vec{k})$$

$$\times Y_H(\vec{v}, (\vec{k}), |\Delta(\vec{k})|, T)/v_1(\vec{k})/v_2(\vec{k})$$

for $\mu = x, y$ where $Y_H(\vec{v}, \Delta, T)$ is the generalized Yosida function,

$$Y_H(\vec{v}, \Delta, T) = \frac{1}{2} \int d\varepsilon f'((\sqrt{\varepsilon^2 + \Delta^2} + \vec{v} \cdot \vec{q}_H/2)$$

$$+ f'((\sqrt{\varepsilon^2 + \Delta^2} - \vec{v} \cdot \vec{q}_H/2)$$

$$\text{(47)}$$

Since $Y_H(\vec{v}, \Delta, 0) = 1/2 (1 - 4\Delta^2/|v_1(\vec{k})|^2)$ for $|\Delta| < |v_1(\vec{k})|/2$, the Doppler shift boosts the differential spin susceptibility in the SC state with a gap node like in CePt$_3$Si.63-65

In Fig. 13 the uniform BCS state is favored at $H = 0$ and the helical SC state is induced by an infinitesimal magnetic field owing to the linear coupling between the magnetization and the helicity $\vec{q}_H$ (eq. (46)) with $\vec{q}_H \perp \vec{H}$. Since the amplitude of $\vec{q}_H$ is linear in the magnetic field $|\vec{H}|$, the formation of helical SC state leads to a correction to the linear response theory in §2 of the uniform state. However, the correction is negligible when $|\alpha| \ll \varepsilon_F$ because the amplitude of $\vec{q}_H$ is small, $|\vec{q}_H| \sim (\alpha/\varepsilon_F) h/v_F$ in linear order of small parameter $\alpha/\varepsilon_F$.

The helicity can play a quantitatively more important role in the non-linear response regime, because the amplitude of $\vec{q}_H$ increases from $|\vec{q}_H| \sim (\alpha/\varepsilon_F) h/v_F$ to the low field region to $|\vec{q}_H| \sim h/v_F$ in the high field region with a rapid crossover around $h \sim T_c$. For example, Fig. 13 shows the magnetic field dependence of the helicity $|\vec{q}_H|$ in the $p$-wave state, with a sharp increase of the helicity above $h = T_c$. As a result the critical field $h_{c2}$ is significantly enhanced at high fields as shown in Figs. 2 and 5.

The nature of the crossover from $|\vec{q}_H| \sim (\alpha/\varepsilon_F) h/v_F$ to $|\vec{q}_H| \sim h/v_F$ becomes obvious observing the momentum dependence of eigenvalues $\lambda(\vec{q})$ in eqs. (40) and (41). Figures 14(a) and (b) show the numerical results in the PM and AFM states, respectively. In Fig. 14(a), $\lambda(\vec{q})$ possesses a crossover from a single to a double peak structure, yielding a rapid increase of the helicity. This result implies that the nature of the helical SC phase is different below and above the crossover magnetic field. Actually, the “stripe SC state” can be stabilized above the crossover field. As shown in Fig. 14(b), the crossover from the single to the double peak structure is suppressed by the AFM order. The eigenvalue $\lambda(\vec{q})$ has a single peak even in the magnetic field much higher than the standard
paramagnetic limit. This is simply because the AFM order suppresses the paramagnetic depairing effect in the p-wave state.

We would like to point here that CePt$_3$Si is a good candidate for an experimental observation of the helical SC phase. Actually, the large critical field $H_{c2}$ leads to the helical SC phase with large $\lambda |\vec{q}| (|\vec{q}| \sim h/v_F)$ in a large part of the $H$-$T$ phase diagram. It seems to be difficult to detect the helical SC phase with small helicity $|\vec{q}| \sim \alpha/\epsilon_v h/v_F$ because the wave length is much longer than the coherence length. Thus the high field phase with $|\vec{q}| \sim h/v_F$ is more promising for the experimental observation. The high field phase is stable in the $p$-wave state above $h = T_c$ as shown in Figs. 4, 10 and 13. However, this phase shrinks in the SC state with dominantly spin singlet pairing and/or the strong orbital depairing effect which leads to small $H_{c2}$.

9. Summary and Discussions

We have investigated the paramagnetic properties in NCSC. The SC states with leading $p$-wave, $d$-wave or $s$-wave order parameter have been examined in view of the heavy Fermion superconductors, CePt$_3$Si, CeRhSi$_3$ and CeIrSi$_3$.

First, the linear response to the magnetic field has been investigated with the particular interest on the role of AFM order. The spin susceptibility is universal in the investigated with the particular interest on the role of CeIrSi$_3$-wave suppression of the paramagnetic depairing effect in the $p$-wave state.

We have proposed several experiments which can provide further evidences for the pairing state in CePt$_3$Si as well as in CeRhSi$_3$ and CeIrSi$_3$. The first proposal is the pressure dependence in various quantities. If the AFM order is a major cause of the unusual properties in CePt$_3$Si, a pronounced pressure dependence is expected in NMR, specific heat, thermal transport, superfluid density and so on. If CePt$_3$Si has a leading $p$-wave order parameter, the following behaviors are expected above
the critical pressure $P \sim 0.6\text{GPa}$. (a) The Knight shift decreases below $T_c$ for the magnetic field along the $ab$-plane and below the standard paramagnetic limit. (b) The paramagnetic depairing effect is enhanced for $H \parallel ab$ but not for $H \parallel c$. (c) The low-energy excitations due to the accidental line nodes are decreased. The coherence peak in NMR $1/T_1T$ is enhanced by the isotropic SC gap. These pressure dependences are not expected in the intra-plane $d$-wave ($d_{x^2-y^2}$ and $d_{xy}$-wave) and $s$-wave states. The pressure dependence (c) is expected also in the inter-plane $d$-wave state and then the additional phase transition occurs in the $P$-T and $H$-T plane.

Another proposal for a future experiment is the 2-fold anisotropy arising from the AFM order. The strong 2-fold anisotropy is expected in the dominantly $p$-wave state while the anisotropy is negligible in the $s$-wave and intra-plane $d$-wave states. In the inter-plane $d$-wave state the strong 2-fold anisotropy is expected near $T = T_c$ but the anisotropy is suppressed at high magnetic fields. The experimental observation of the 2-fold anisotropy in the AFM state could provide an important evidence for the pairing symmetry in CePt$_3$Si, CeRhSi$_3$ and CefSi$_3$. Thus, the response to the AFM order can be a signature of the pairing symmetry in non-centrosymmetric superconductors.

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Appendix A: Linear Response Theory

The dynamical spin susceptibility in the linear response regime is obtained by the Kubo formula as,

$$\chi^{\mu\nu}(q) = -\sum_{\gamma,\delta} \sum_k \int \frac{d^2 q}{(2\pi)^2} S^{\mu}_{\gamma\delta}(\hat{k} + q, \hat{k}) S^{\nu}_{\gamma\delta}(\hat{k}, \hat{k} + q) G_{\delta}(k + q) G_{\gamma}(k)$$

$$- S^{\mu}_{\gamma\delta}(\hat{k} + q, \hat{k} + q) S^{\nu}_{\gamma\delta}(\hat{k}, \hat{k} + q - \hat{q} - \hat{q}) F_{\delta}(k + q) F_{\gamma}^{\dagger}(k),$$

where $q = (\vec{q}, i\Omega_n)$, $k = (\vec{k}, i\omega_n)$ and $\vec{q}$ is the momentum along the $ab$-plane. The spin operator $S^{\mu}_{\gamma\delta}(\hat{k} + q, \hat{k})$ in the band basis has been given in eq. (17).

Taking the limit $\Omega_n \rightarrow 0$ and $q \rightarrow 0$, we obtain the uniform spin susceptibility $\chi^{\mu\nu} = \lim_{\vec{q} \rightarrow 0} \lim_{\Omega_n \rightarrow 0} \chi^{\mu\nu}(q)$ which can be decomposed into a Van-Vleck and Pauli part as,

$$\chi^{\nu\mu} = \lim_{\vec{q} \rightarrow 0} \lim_{\Omega_n \rightarrow 0} \chi^{\nu\mu}(q),$$

$$\chi^{\mu\nu} = \chi^{\mu\nu} - \chi^{\nu\mu}. \quad (A-3)$$

We obtain the following expressions,

$$\chi^{\mu\nu} = -\lim_{\vec{q} \rightarrow 0} \lim_{\Omega_n \rightarrow 0} \sum_k \int \frac{d^2 q}{(2\pi)^2} S^{\mu}_{\gamma\delta}(\hat{k} + q, \hat{k}) S^{\nu}_{\gamma\delta}(\hat{k}, \hat{k} + q) G_{\delta}(k + q) G_{\gamma}(k)$$

$$- S^{\mu}_{\gamma\delta}(\hat{k} + q, \hat{k} + q) S^{\nu}_{\gamma\delta}(\hat{k}, \hat{k} + q - \hat{q} - \hat{q}) F_{\delta}(k + q) F_{\gamma}^{\dagger}(k),$$

$$\chi^{\nu\mu} = -\sum_{\gamma,\delta,\bar{\gamma}} \sum_k \int \frac{d^2 q}{(2\pi)^2} S^{\mu}_{\gamma\delta}(\hat{k} + q, \hat{k}) S^{\nu}_{\gamma\delta}(\hat{k}, \hat{k} + q) G_{\delta}(k) G_{\gamma}(k)$$

$$- S^{\mu}_{\gamma\delta}(\hat{k} + q, \hat{k} + q) S^{\nu}_{\gamma\delta}(\hat{k}, \hat{k} + q - \hat{q} - \hat{q}) F_{\delta}(k + q) F_{\gamma}^{\dagger}(k).$$

Assuming $|\Delta_{\gamma}(\vec{k})|, \nu_{\nu} |\bar{q}| / 2 \ll |\alpha|$ where $\nu_{\nu}$ is the Fermi velocity, the Van-Vleck part of spin susceptibility eq. (A.5) is obtained as in eq. (16).

When we restrict to the AFM moment along the principal axis, namely $\hat{H}_Q \parallel \hat{x}, \hat{y} \parallel \hat{z}$, the relation $U(-k) = e^{i\theta} \hat{U}(\vec{k})$ holds with $\theta$ an arbitrary phase factor. Here we denote

$$\hat{i} = \left( \begin{array}{cc} \hat{i}_x & 0 \\ 0 & \pm \hat{i}_y \end{array} \right), \quad (A-6)$$

$$\hat{i}_x = \left( \begin{array}{cc} 0 & 1 \\ 1 & 0 \end{array} \right). \quad (A-7)$$

The sign of $\hat{i}_2$ in $\hat{i}$ is $+$ for $\hat{H}_Q \parallel \hat{x}, \hat{y}$ and $-$ for $\hat{H}_Q \parallel \hat{z}$. According to eqs. (17) and (18), we obtain $S^{\mu}_{\gamma\delta}(\hat{k}, \hat{k}) = - S^{\mu}_{\gamma\delta}(\hat{k}, \hat{k})$ for $\mu = x, y$ and $S_{\gamma\delta}^{\mu}(\hat{k}, \hat{k}) = S_{\gamma\delta}^{\mu}(\hat{k}, \hat{k})$. If $v_{\nu} |\bar{q}| / 2 \ll |\alpha|$, the coefficient in eq. (A.4) is approximated as $S^{\mu}_{\gamma\delta}(\hat{k} + \vec{q}, \hat{k} + \vec{q}) \sim S^{\mu}_{\gamma\delta}(\hat{k}, \hat{k}) S^{\mu}_{\gamma\delta}(\hat{k} - \hat{q}, \hat{k} - \hat{q})$ and the Pauli part of spin susceptibility is obtained as eq. (15).

Appendix B: Magnetic Properties in the $d$-wave State

For the discussion for the intra-plane $d$-wave state we adopt the model eq. (29) but assume the tight binding parameters in eq. (27) as,

$$(t_1, t_4, n) = (1, 0.2, 0.8), \quad (B-1)$$

with all other parameters zero. This parameter set leads to the nearly half-filled band with quasi-two-dimensional Fermi surface and leads to the dominantly $d_{x^2-y^2}$-wave SC state for the parameter set (A) $U > 0, V = -0.8U$. The order parameters are described as $\Phi(\vec{k}) = \delta + \eta \cos k_x - \cos k_y$ with $\delta = 0$ and $\eta = 1$ at $h_Q = h = 0$. Our analysis confirms $|\delta|, |1 - \eta| \ll 1$. In general, the $d_{x^2-y^2}$-wave state is admixed with the $f_{x}(x^2-y^2)$- and $f_{y}(x^2-y^2)$-wave order parameters owing to the SOC. However, the $f$-wave component does not appear in the mean field solution of the effective model eq. (29) because interactions beyond the nearest neighbor sites are neglected.

We calculate the critical magnetic field $h_{c2}$ by solving the linearized mean field equation eqs. (40) and (41) and show the result in Fig. 4. The spin susceptibility is calculated on the basis of eq. (43) by solving the mean field equation eqs. (35-38). In Fig. B.1 we show the spin susceptibility below $T_c$ for various magnetic fields. These results should be contrasted to those for the $p$-wave state (Figs. 4, 6, 10 and 11).
Fig. B.1. (Color online) The spin susceptibility along the [100]- and [010]-directions in the d-wave state without AFM order. We assume $U > 0$, $V = -0.8U$, $J = 0$, $\alpha = 0.3$ and $bQ = 0$. The magnetic field is chosen as $h = 0.1T_c$, $h = T_c$, $h = 1.5T_c$, and $h = 2T_c$ from the bottom to the top.

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