## Theory of parity-violated Cooper pairs in weakly noncentrosymmetric superconductors

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We propose that in noncentrosymmetric superconductors with *weakly* asymmetric spin-orbit interaction, the field-induced pair correlation between the spin-orbit split different bands ignored in previous studies yields unique effects; i.e., the Pauli depairing effect is anisotropic in the momentum space and, as a result, magnetic fields induce a point-node-like anisotropic gap structure of the quasiparticle energy even for isotropic *s*-wave states, which seriously affects thermodynamic quantities at low temperatures. Also, it is shown that when the magnitude of the spin-orbit interaction is smaller than the superconducting gap, the specific heat as a function of the magnetic field exhibits a two-gap-like behavior, even when there is only a single gap. These features characterize parity-violated Cooper pairs in weakly noncentrosymmetric systems. We suggest the possible detection of these effects in the superconductor with weakly broken inversion symmetry  $Y_2C_3$ .

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# I. INTRODUCTION

One of the intriguing features of the recently discovered noncentrosymmetric superconductors<sup>1-5</sup> is the realization of parity-violated Cooper pairs, which lead various exotic phenomena.<sup>6–22</sup> The investigations for unique effects characterizing parity violation have been mainly focused on the case with strongly broken inversion symmetry (IS), where the spin-orbit (SO) band splitting  $E_{SO}$  is enormous compared to the superconducting (SC) gap  $\Delta$ , because it is commonly believed, and partly true, that effects due to broken IS are more prominent for stronger SO interaction. However, in the present paper, we propose the possibility of other phenomena which characterize parity-violated Cooper pairs in a unique way inherent in *weakly* noncentrosymmetric systems. These phenomena are essentially raised by the Zeeman effect on pairing states in the SO split two bands. In the weakly noncentrosymmetric case  $E_{SO} \sim \Delta$ , the Zeeman magnetic field induces substantial pair correlation between the SO split different bands competing with the intraband pairs, which is, in contrast, negligible in strongly noncentrosymmetric systems with  $E_{SO} \ge \Delta$ .<sup>6,14–16,18–20</sup> We demonstrate that the fieldinduced interband pair correlation changes drastically lowenergy properties of the SC state in the case with weakly broken IS, yielding the following unique effects: (i) the Pauli depairing effect is anisotropic in the momentum space and, as a result, magnetic fields induce the point-node-like structure of the excitation gap even for isotropic s-wave states, which seriously affects thermodynamic quantities, yielding distinct behaviors of them at low temperatures. (ii) For  $E_{SO}$  $<\Delta$ , the specific heat as a function of magnetic fields exhibits a two-gap-like behavior even when there is only a single SC gap. These effects are associated with the momentumdependent spin orientation of Cooper pairs which characterizes parity violation. Thus, our results suggest another possible direction of the experimental search for parity-violated Cooper pairs.

As a matter of fact, our findings are relevant to the recent experimental studies on the weakly noncentrosymmetric superconductor  $Y_2C_3$ .<sup>25–28</sup> This system has a cubic crystal structure with the space group symmetry  $I\bar{4}3d$  breaking in-

version symmetry. Thus, the asymmetric SO interaction can be approximated by the Dresselhaus type interaction. The unique feature of this system is that the SO splitting is almost of the same order as the superconducting gap,<sup>29,30</sup> and thus, the situation considered in the present paper may be realized in this material. In the last part of this paper, we shall compare our results with the experimental observations for this system and discuss the possible realization of the distinct phenomena characterizing parity-violated Cooper pairs in  $Y_2C_3$ .

Although the existence of the indispensable interband pairing correlation, in addition to the intraband pairs mentioned above, plays an essential role in the above unique phenomena, it also brings about some technical complexity of theoretical treatment which hinders the elucidation of properties of weakly noncentrosymmetric superconductors. Moreover, the magnetic field induces the orbital depairing effect as well as the Zeeman effect mentioned above. To deal with these issues, we first analyze exactly the effects of the Zeeman magnetic field on the quasiparticle energy, neglecting the orbital depairing effect, and, afterward, to take into account the orbital effect, we develop the quasiclassical method which extends the classical works by Eilenberger<sup>23</sup> and Larkin-Ovchinnikov<sup>24</sup> to the case with both the intraband and interband pairs. A similar quasiclassical approach was considered before by Hayashi et al.21 Here, we obtain the explicit analytical solutions of the Eilenberger equations which encompass both the intraband and interband pairs. Using them, we discuss the behaviors of thermodynamic quantities under an applied magnetic field, in which the abovementioned unique features characterizing parity-violated Cooper pairs appear.

The organization of this paper is as follows. In Sec. II, we investigate the Zeeman field effect in a weakly noncentrosymmetric superconductor with the Dresselhaus type SO interaction, neglecting the orbital depairing effect, and demonstrate that in the case of  $E_{SO} \sim \Delta$ , the Pauli depairing effect is anisotropic in the momentum space, leading to the point-node-like anisotropic structure of the excitation energy gap. This phenomenon should be important in the mixed state of type II superconductors. Thus, in Sec. III, we develop the quasiclassical method, taking into account the orbital depair-

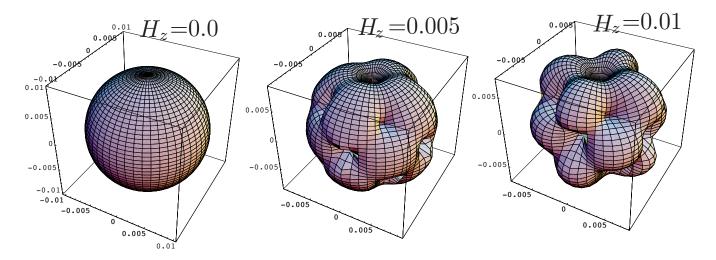


FIG. 1. (Color online) The structure of the single-particle excitation energy gap on the spherical Fermi surface of the band  $\varepsilon_{k-}$  for  $H_z=0.0, 0.005$ , and 0.01.

ing effect in addition to the above-mentioned anisotropic Pauli depairing effect. Based on this method, in Sec. IV, we investigate the thermodynamic properties of the mixed state and elucidate how the above features characterizing the parity-violated Cooper pairs appear in experimentally observable quantities. It is demonstrated that for a sufficiently small SO interaction,  $E_{SO} < \Delta$ , the specific heat as a function of magnetic fields exhibits a two-gap-like behavior even when there is only a single SC gap. We shall also discuss the implication of our results for the recent experimental researches on the weakly noncentrosymmetric superconductor  $Y_2C_3$ .<sup>25–28</sup> A summary is given in Sec. V.

## **II. ANISOTROPIC PAULI DEPAIRING EFFECT**

The absence of the inversion symmetry is characterized by the asymmetric SO interaction,

$$\mathcal{H}_{\rm SO} = \alpha \sum_{k,\sigma,\sigma'} \mathcal{L}_0(k) \cdot \boldsymbol{\sigma}_{\sigma\sigma'} c_{k\sigma}^{\dagger} c_{k\sigma'}, \qquad (1)$$

where  $c_{k\sigma}$  ( $c_{k\sigma}^{\mathsf{T}}$ ) is the annihilation (creation) operator of an electron with momentum *k* and spin  $\sigma$ . The components of  $\boldsymbol{\sigma} = (\sigma^x, \sigma^y, \sigma^z)$  are the Pauli matrices. Since we are concerned with the application to the cubic system Y<sub>2</sub>C<sub>3</sub> with the space group symmetry  $I\bar{4}3d$ , we assume the Dresselhaus interaction,  $\mathcal{L}_0(k) = (\mathcal{L}_{0x}, \mathcal{L}_{0y}, \mathcal{L}_{0z}) = [k_x(k_y^2 - k_z^2), k_y(k_z^2 - k_x^2), k_z(k_x^2 - k_y^2)].^{31}$ 

In the following, we consider the case of an *s*-wave state with the isotropic SC gap  $\Delta$ , for which the features of weakly broken IS appear profoundly, as shown below. We ignore the admixture with triplet pairs, which is justified for  $E_{\rm SO}/E_{\rm F} \ll 1$ . Our model Hamiltonian reads,

$$\mathcal{H} = \mathcal{H}_{BCS} + \mathcal{H}_{SO}, \tag{2}$$

$$\mathcal{H}_{\text{BCS}} = \sum_{k,\sigma} \varepsilon_k c_{k\sigma}^{\dagger} c_{k\sigma} - \sum_k \left[ \Delta c_{k\uparrow}^{\dagger} c_{-k\downarrow}^{\dagger} + \Delta^* c_{-k\downarrow} c_{k\uparrow} \right].$$
(3)

In the following, the spherical Fermi surface,  $\varepsilon_k = k^2/2m$ - $E_F$ , is assumed for simplicity. In this section, we concen-

trate on the effects of the Zeeman interaction, expressed by  $-\Sigma_{k,\sigma\sigma'}\mu_B \boldsymbol{H} \cdot \boldsymbol{\sigma}_{\sigma\sigma'} c_{k\sigma}^{\dagger} c_{k\sigma'}$ , with  $\boldsymbol{H} = (0,0,H_z)$ , leaving the analysis of the orbital depairing effect until the next sections. When the Zeeman term is added to the Hamiltonian (2), the magnetic field induces the pairing between electrons on the SO split different bands, which gives rise to the Pauli depairing effect. The important observation is that in the case of  $E_{\rm SO} \sim \Delta$ , Cooper pairs with **k** for which the spin degeneracy is not lifted by the SO interaction are more seriously affected by the Pauli depairing effect than electron pairs in the strongly SO split regions, leading to the anisotropic Pauli depairing in the momentum space. The anisotropic Zeeman effect in the strongly noncentrosymmetric case has already been discussed by several authors.<sup>10,17</sup> The unique point in the weakly noncentrosymmetric case is that this effect drastically changes the structure of low-energy excitations in the SC state and yields the point-node-like structure of the single-particle excitation gap even in isotropic *s*-wave states. To demonstrate this, we calculate the single-particle excitation energy  $E_{k\mu}$  ( $\mu$ =1, 2, 3, and 4) by diagonalizing the above mean field Hamiltonian (2) with the Zeeman term expressed in the  $4 \times 4$  matrix form in the space spanned by the basis  $(c_{k\uparrow}^{\dagger}, c_{-k\uparrow}, c_{k\downarrow}^{\dagger}, c_{-k\downarrow})$ . The explicit expressions for  $E_{k\mu}$  are given in Appendix A. In Fig. 1, we depict the numerically calculated single-particle excitation energy gap  $E_{gap}$  for the band  $\varepsilon_{k-} \equiv \varepsilon_k - |\alpha \mathcal{L}_0(\mathbf{k}) - \mu_B \mathbf{H}|$  in the case with  $\Delta / E_F = 0.01$ and  $\alpha/E_F=0.03$ . Here,  $E_{gap}$  is defined by the magnitude of  $E_{k3}$  for k on the Fermi surface satisfying  $\varepsilon_{k-}=0$ . It is seen that the point-node-like structure develops as the magnetic field increases. As a matter of fact, the excitation energy  $E_{k\mu}$ is not truly gapless, but the excitation energy gap  $E_{gap}$  is strongly anisotropic, with the structure similar to the point nodes, reflecting the k dependence of the SO term even when the superconducting gap  $\Delta$  is independent of k. For instance, the excitation energy gaps  $E_{gap}$  for  $\mathbf{k}_F || (001), \mathbf{k}_F || (111)$ , and  $\mathbf{k}_F \| (100)$  [equivalent to  $\mathbf{k}_F \| (010) \|$  are equal and given by

$$E_{\rm gap}^{(001)} = E_{\rm gap}^{(111)} = E_{\rm gap}^{(100)} = \sqrt{(\mu_B H_z)^2 + \Delta^2} - \mu_B H_z, \qquad (4)$$

while for  $\boldsymbol{k}_F \| (110)$ ,

$$E_{\rm gap}^{(110)} \approx \sqrt{2f(H_z) + \Delta^2 - 2\sqrt{f(H_z)^2 + \mu_B^2 H_z^2 \Delta^2}}, \qquad (5)$$

with  $f(H_z)=2\alpha^2 k_F^6 + \mu_B^2 H_z^2$ . It is easily checked that  $E_{gap}^{(110)} > E_{gap}^{(001)}$ . The positions of the gap minima coincide approximately with the zero points of  $\mathcal{L}_0(\mathbf{k})$  at which the SO splitting vanishes. The quasiparticle excitations for  $\mathbf{k}_F || (001)$ , (111), and (100) behave like Dirac fermions, with the mass gap given by Eq. (4). It should be stressed that in the situation considered here, the single-particle energy gap  $E_{gap}$  does not coincide with the superconducting gap  $\Delta$ , which is k independent. A similar anisotropic structure of the excitation gap also appears for the band  $\varepsilon_{k+} \equiv \varepsilon_k + |\alpha \mathcal{L}_0(\mathbf{k}) - \mu_B \mathbf{H}|$ .

Although we use the Dresselhaus interaction in the present calculation, the point-node-like structure appears generally for any forms of  $\mathcal{L}_0(k)$  which possess zero points on the Fermi surface.

## III. QUASICLASSICAL APPROACH FOR THE MIXED STATE IN THE CASE WITH BOTH INTERBAND AND INTRABAND PAIRINGS

The anisotropic Pauli depairing effect discussed in the previous section is particularly important in type II superconductors. Thus, in the following, we consider the orbital depairing effect as well as the Pauli depairing effect on the basis of the quasiclassical analysis. For this purpose, we consider the Green functions for quasiparticles defined on the SO split bands,  $G^{(\mu\nu)}(x,x') = -\langle T_\tau \psi_{\mu}(x)\psi_{\nu}^{\dagger}(x')\rangle$  and  $F^{(\mu\nu)}(x,x') = -\langle T_\tau \psi_{\mu}^{\dagger}(x)\psi_{\nu}^{\dagger}(x')\rangle$ , where  $\psi_{\mu}(x)$  and  $\psi_{\mu}^{\dagger}(x)$  are the field operators for quasiparticles in the  $\mu$  band corresponding to the energy in the normal state  $\varepsilon_{k\mu} = \varepsilon_k + \mu \alpha |\mathcal{L}_0(k)|$ , with  $\mu = \pm$ .<sup>32</sup> As mentioned above, the interband Green functions. Fourier transforming  $G^{(\mu\nu)}$  and  $F^{(\mu\nu)}$ , we introduce the quasiclassical Green functions defined by

$$\hat{\mathcal{G}}(\hat{k}, \boldsymbol{r}, \boldsymbol{\varepsilon}_n) = \begin{pmatrix} g^{(++)} & -f^{(++)} & g^{(+-)} & -f^{(+-)} \\ f^{(++)} & \overline{g}^{(++)} & f^{(-+)\dagger} & \overline{g}^{(-+)} \\ g^{(-+)} & -f^{(-+)} & g^{(--)} & -f^{(--)} \\ f^{(+-)\dagger} & \overline{g}^{(+-)} & f^{(--)\dagger} & \overline{g}^{(--)} \end{pmatrix}, \quad (6)$$

with  $g^{(\mu\nu)}(\hat{k}, \boldsymbol{r}, \varepsilon_n) = \int (d\varepsilon_k / \pi) G^{(\mu\nu)}(\boldsymbol{k}, \boldsymbol{r}, \varepsilon_n), \quad f^{(\mu\nu)}(\hat{k}, \boldsymbol{r}, \varepsilon_n) = \int (d\varepsilon_k / \pi) F^{(\mu\nu)}(\boldsymbol{k}, \boldsymbol{r}, \varepsilon_n), \text{ and } \overline{g}^{(\mu\nu)} = g^{(\mu\nu)}(-k, \boldsymbol{r}, -\varepsilon_n).$  Here,  $\boldsymbol{k}$  is the momentum conjugate to the relative coordinate  $\boldsymbol{x} - \boldsymbol{x}', \boldsymbol{r}$  is the center of mass coordinate,  $\hat{k}$  is a unit vector parametrizing the direction of momentum  $\boldsymbol{k}$ , and  $\varepsilon_n$  is the fermionic Matsubara frequency. Hereafter, matrices  $\breve{A}$  represent  $2 \times 2$  matrices defined in the space spanned by the basis  $(\psi_{\mu}, \psi_{\nu}^{\dagger}),$  where  $\mu = \nu = \pm$  or  $\mu = -\nu = \pm$ , and matrices  $\widetilde{B}$  represent those in the two-dimensional space spanned by the band indices + and -. Using the standard method, <sup>23,24,33</sup> we find that  $\hat{\mathcal{G}}$  satisfies the Eilenberger equation in the clean limit,

$$i\boldsymbol{v}\cdot\frac{\partial}{\partial \boldsymbol{r}}\hat{\mathcal{G}}+[\omega\tau^{z}-\hat{M}+\hat{\Delta},\hat{\mathcal{G}}]=0, \qquad (7)$$

where  $\omega = 2i\varepsilon_n + \mathbf{v} \cdot \frac{2e}{c} \mathbf{A}$ , with  $\mathbf{A}$  a vector potential, and  $\tau^z = \tilde{1} \otimes \breve{\sigma}^z$ . The  $4 \times 4$  matrix  $\hat{M}$  is defined by  $\hat{M}(\hat{k}) = \breve{\sigma}^z \otimes (\alpha \breve{L}(\hat{k}))$ , where  $\breve{L}(\hat{k}) = \breve{1}(|\mathcal{L}(\hat{k})| + |\mathcal{L}(-\hat{k})|)/2 + \breve{\sigma}^z(|\mathcal{L}(\hat{k})| - |\mathcal{L}(-\hat{k})|)/2$  and  $\alpha |\mathcal{L}(\hat{k})| = |\alpha \mathcal{L}_0(\hat{k}) - \mu_B \mathbf{H}|$ . The matrix gap function  $\hat{\Delta}(\hat{k}, \mathbf{r})$  is

$$\hat{\Delta}(\hat{k},\boldsymbol{r}) = \begin{pmatrix} \breve{\Delta}_{+}(\hat{k},\boldsymbol{r}) & \breve{\Delta}_{2}(\hat{k},\boldsymbol{r}) \\ -\breve{\Delta}_{2}(\hat{k},\boldsymbol{r}) & \breve{\Delta}_{-}(\hat{k},\boldsymbol{r}) \end{pmatrix},$$
(8)

with  $\check{\Delta}_{\pm}(\hat{k}, \mathbf{r}) = i\check{\sigma}_{y} \operatorname{Re} \Delta_{\pm}(\hat{k}, \mathbf{r}) + i\check{\sigma}_{x} \operatorname{Im} \Delta_{\pm}(\hat{k}, \mathbf{r}), \quad \check{\Delta}_{2}(\hat{k}, \mathbf{r})$   $= \check{\sigma}_{x} \operatorname{Re} \Delta_{2}(\hat{k}, \mathbf{r}) - \check{\sigma}_{y} \operatorname{Im} \Delta_{2}(\hat{k}, \mathbf{r}), \qquad \Delta_{\pm}(\hat{k}, \mathbf{r}) = \Delta(\mathbf{r})s_{\pm}(\hat{k}),$  $\Delta_{2}(\hat{k}, \mathbf{r}) = \Delta(\mathbf{r})s_{2}(\hat{k}), \text{ and}$ 

$$s_{\pm}(\hat{k}) = -\left[\xi_{+}(\hat{k})\xi_{-}(-\hat{k}) + \xi_{-}(\hat{k})\xi_{+}(-\hat{k})\right]\eta_{\pm}(\hat{k}), \qquad (9)$$

$$s_2(\hat{k}) = \xi_+(\hat{k})\xi_+(-\hat{k}) - \xi_-(\hat{k})\xi_-(-\hat{k}), \qquad (10)$$

where  $\xi_{\pm}(\hat{k}) = \sqrt{(1 \pm \mathcal{L}_z(\hat{k}) | \mathcal{L}(\hat{k})|)/2}$  and  $\eta_{\pm}(\hat{k}) = -(\mathcal{L}_x \pm i\mathcal{L}_y)/\sqrt{\mathcal{L}_x^2 + \mathcal{L}_y^2}$ . Here, we omit the corrections to the Fermi velocity from the SO interaction, which are not important for  $E_{\text{SO}}/E_{\text{F}} \ll 1$ . In the case with strong SO interaction  $\alpha \gg \Delta$ , the contributions from the interband Green functions to Eq. (7) are negligible and the two bands are decoupled. This simplified case was previously studied by several authors.<sup>21,22</sup>

In spite of the complications raised by the existence of both the interband and intraband Green functions, the analytical solutions of Eq. (7) based on the Pesch type approximation are possible. In this approach, we assume the Abrikosov lattice solution for  $\Delta(\mathbf{r})$  and the uniform magnetic field in the system, and replace the normal Green functions  $g^{(\mu\nu)}$ and  $\overline{g}^{(\mu\nu)}$  with the spatial averages over a unit cell of the vortex lattice,  $\langle g^{(\mu\nu)} \rangle$  and  $\langle \overline{g}^{(\mu\nu)} \rangle$ , retaining only the spatial variation of  $f^{(\mu\nu)}$  and  $f^{(\mu\nu)\dagger}$ . Utilizing the normalization condition  $\hat{\mathcal{G}} \cdot \hat{\mathcal{G}} = \mathbf{1}$  and the relations  $\operatorname{tr}[\hat{\mathcal{G}}] = 0$  and  $g^{(+-)*} = g^{(-+)}$ , which are derived from Eq. (7),<sup>35</sup> we find that the quasiclassical Green functions are given by the solutions of the coupled algebraic equations,

$$\sum_{\nu=\pm} |\langle g^{(\mu\nu)} \rangle|^2 - \sum_{\sigma,\nu=\pm} P(\tilde{\varepsilon}_n^{(\sigma\nu)}) |s_{\sigma\nu} \langle g^{(\sigma \ \nu\sigma)} \rangle - s_{\sigma} \langle \bar{g}^{(\nu\sigma \ \sigma)} \rangle - \nu \sigma s_2 (\langle g^{(\sigma \ -\nu\sigma)} \rangle + \nu \langle \bar{g}^{(\nu\sigma \ -\sigma)} \rangle)|^2 = -1 \quad (\mu = \pm),$$
(11)

$$\langle g^{(+-)} \rangle = C \sum_{\mu,\nu=\pm} \nu [Y(\tilde{\varepsilon}_n^{(\mu\nu)}) \langle g^{(\mu\mu)} \rangle - Y(\tilde{\varepsilon}_n^{(\nu\mu \ \nu)}) \langle \bar{g}^{(\mu\mu)} \rangle],$$
(12)

where  $\tilde{\varepsilon}_n^{(\mu\nu)} = \varepsilon_n + \frac{i\alpha\mu}{2} (|\mathcal{L}| - \nu |\mathcal{L}'|), \quad \mathcal{L}' = \mathcal{L}(-\hat{k}), \quad P(\varepsilon)$ =  $\frac{1}{2} \partial Y(\varepsilon) / \partial \varepsilon$ , and  $Y(\tilde{\varepsilon}_n) = \sqrt{\pi} \Delta^2 u_n W(2iu_n \tilde{\varepsilon}_n)$ , with  $\Delta^2 = \langle \Delta^2(\mathbf{r}) \rangle, \quad W(z) = e^{-z^2} \operatorname{erfc}(-iz), \text{ and } u_n = \Lambda \operatorname{sgn} \varepsilon_n / v \sin \theta,$ with  $\Lambda = \sqrt{\hbar c / 2eH_z}$  and  $\theta$  the polar angle of  $\hat{k}$ , and  $C = 2is_2 s_+ \alpha |\mathcal{L}'| / \tilde{D}$  with

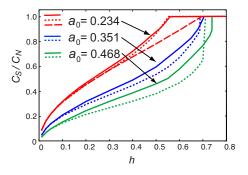


FIG. 2. (Color online) Specific heat at  $T=0.1T_c$  divided by the normal state value  $C_N$  as a function of the normalized magnetic field  $h=\mu_B H_z/\Delta_0$  for  $\alpha/\Delta_0=1.0$  (solid line),  $\alpha/\Delta_0=0.0$  (dotted line), and  $\alpha/\Delta_0=10.0$  (dashed line).

$$\widetilde{D} = 4\alpha^{2}|\mathcal{L}||\mathcal{L}'| + 2i|s_{+}|^{2}\alpha(|\mathcal{L}| + |\mathcal{L}'|)\sum_{\mu=\pm}\mu Y(\widetilde{\varepsilon}_{n}^{(\mu-)})$$
$$- 2is_{2}^{2}\alpha(|\mathcal{L}| - |\mathcal{L}'|)\sum_{\mu=\pm}\mu Y(\widetilde{\varepsilon}_{n}^{(\mu+)}).$$
(13)

Since the explicit expressions of the solutions are lengthy, we will present them in Appendix B and, instead, concentrate on the discussion on the results obtained from them in the following section.

### IV. SPECIFIC HEAT COEFFICIENT AND DENSITY OF STATES

Using the analytical solutions for  $\hat{\mathcal{G}}$ , we calculate the specific heat and the density of states of quasiparticles. For this purpose, we determine the field dependence and the temperature dependence of the spatially averaged gap function  $\Delta(H_z,T) = \sqrt{\langle \Delta^2(\mathbf{r}) \rangle}$  by solving the quasiclassical BCS gap equation,

$$\langle \Delta^2(\boldsymbol{r}) \rangle = \lambda_0 T \sum_n \sum_{\hat{k}} \langle \Delta(\boldsymbol{r}) f_{\uparrow\downarrow}(\hat{k}, \boldsymbol{r}, \boldsymbol{\varepsilon}_n) \rangle, \qquad (14)$$

$$f_{\uparrow\downarrow} = \xi_{-}\overline{\xi}_{-}f^{(-+)} + \xi_{+}\overline{\xi}_{+}f^{(+-)} - \xi_{+}\overline{\xi}_{-}f^{(++)} - \xi_{-}\overline{\xi}_{+}f^{(--)}, \quad (15)$$

where  $\overline{\xi}_{\alpha} \equiv \xi_{\alpha}(-k)$ .  $\lambda_0$  is a dimensionless coupling constant. To compare our calculated results with the experimental observations for Y<sub>2</sub>C<sub>3</sub> later, we tune the values of  $\lambda_0$  and the cutoff for the frequency sum  $\varepsilon_c$  so as to realize  $T_c=18$  K (e.g.,  $\lambda_0=0.2703$  and  $\varepsilon_c=700$  K). In this calculation, an important parameter is  $a_0 \equiv \sqrt{\mu_B \hbar c/2e \Delta_0}/\pi \xi_0$ , which is an inverse of the coherence length  $\xi_0$  normalized to be dimensionless. Here,  $\Delta_0$  is the gap function for  $H_z=0$ . For Y<sub>2</sub>C<sub>3</sub>,  $a_0 \approx 0.234$ . The specific heat in the SC state is

$$C_{S} = \int d\varepsilon \frac{\varepsilon^{2}}{4T^{2} \cosh^{2}(\varepsilon/2T)} D_{S}(\varepsilon), \qquad (16)$$

where the density of states for quasiparticles  $D_S(\varepsilon)$  is given by  $D_S(\varepsilon) = D_N(0) \Sigma_k \Sigma_{\mu=\pm} \operatorname{Im} \langle g^{(\mu\mu)}(\hat{k}, \boldsymbol{r}, \varepsilon + i\delta) \rangle$ , with  $D_N(0)$ the density of states in the normal state. In Fig. 2, we present the calculated results of the specific heat as a function of the

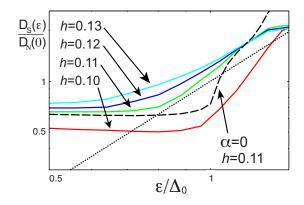


FIG. 3. (Color online) Log-log plot of the density of states versus energy for  $\alpha/\Delta_0=1.0$ . The density of states for  $\alpha=0.0$  and h=0.11 is also shown for comparison (broken line). The dotted line is  $\varepsilon^2$ .

normalized magnetic field  $h = \mu_B H_z / \Delta_0$  for the temperature  $T/T_c = 0.1$  and several sets of the parameters  $\alpha / \Delta_0$  and  $a_0$ . It is found that in contrast to the case with strongly broken IS where the SC state is quite robust against the Pauli depairing effect, in weakly noncentrosymmetric systems, more low-energy excitations are induced by the magnetic field than in the case with inversion symmetry  $\alpha = 0$ . We interpret the origin of this behavior as the existence of the field-induced nodal excitations mentioned above. The emergence of the point-node-like excitations is more clearly observed in the energy dependence of the density of states for quasiparticles, which is plotted in Fig. 3 for  $\alpha / \Delta_0 = 1.0$ . As the magnetic field increases, the density of states exhibits the power-law behavior  $D_s(\varepsilon) \propto \varepsilon^2$ .

When the SO coupling  $\alpha$  is sufficiently smaller than  $\Delta_0$ , another remarkable feature appears in the field dependence of the specific heat. As shown in Fig. 4, for the low magnetic fields  $h \approx 0.1-0.2$ , a shoulderlike structure of  $C_S(H_z)$  similar to a two-gap behavior appears, though there is only a single SC gap  $\Delta(\mathbf{r})$ . The origin of this behavior is understood as follows. For  $\alpha < \Delta_0$ , there are two different types of the Pauli depairing effect, i.e., (i) one due to the generation of the interband pairing correlation, which, instead, suppresses the intraband pairing, and (ii) the other caused by the asymmet-

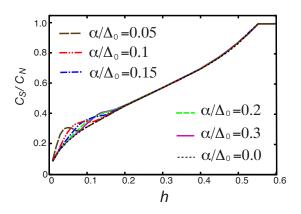


FIG. 4. (Color online) Specific heat as a function of the normalized magnetic field *h* for small  $\alpha/\Delta_0$ .  $a_0=0.234$  and  $T=0.1T_c$ .

ric deformation of the Fermi surface. The former is analogous to the usual Pauli depairing effect in centrosymmetric superconductors. The latter effect is inherent in noncentrosymmetric systems. The crucial point is that although the former exists for any finite magnetic fields, the latter is effective only for small fields  $\mu_B H_z < \alpha$  and is suppressed for larger fields  $\mu_B H_z > \alpha$ . As a result, the character of the Pauli depairing effect changes around  $H_z \sim \alpha/\mu_B$  in the case of  $\alpha$  $<\Delta_0$ , yielding the shoulder structure of the specific heat coefficient as demonstrated in Fig. 4. We would like to stress that this effect is caused by the momentum-dependent spin orientation of Cooper pairs characterizing parity violation. Three remarks are in order. (1) For sufficiently small  $\alpha$ , e.g.,  $\alpha$ =0.05, C<sub>S</sub> exhibits a hump rather than a shoulder, in marked contrast with conventional two-gap behaviors. (2) As  $\alpha$  increases, the position of the shoulder shifts to larger h regions, though its structure becomes obscure since the orbital depairing effect dominates for high magnetic fields. (3) It should be cautioned that the Pesch approximation is not valid for magnetic fields much lower than  $H_{c2}$ .<sup>33,34</sup> However, the shoulder structure of  $C_s$  at  $h \sim 0.1$  stems from the Zeeman effect rather than from orbital depairing effects. Thus, the above results are applicable to systems with a sufficiently large value of the Ginzburg-Landau parameter  $\kappa$ , where small magnetic fields can penetrate deeply into the SC regions.

We, now, discuss the implication of the above results for the experimental observations of the weakly noncentrosymmetric superconductor  $Y_2C_3$ . This system is almost in the London limit with  $\kappa > 10.^{25,27}$  According to the recent localdensity approximation calculation, the averaged magnitude of the SO band splitting is roughly  $\sim 0.01 \text{ eV},^{30}$  which is of the same order as the SC gap  $\sim 30 \text{ K}.^{27}$  Thus, our analysis is applicable. A remarkable experimental observation for  $Y_2C_3$ is that the field dependence of the specific heat exhibits a small shoulder structure for  $H_z \sim 8 \approx H_{c2}/3$  T at  $T=2.6 \text{ K}.^{28}$ Although this behavior was interpreted as the indication of the existence of two SC gaps with different magnitudes,<sup>26,28</sup> it can be also, alternatively, explained by assuming the realization of the unique effect associated with parity violation as demonstrated in Fig. 4. A possible test for our scenario is to investigate the field dependence of the nuclear spin relaxation rate,<sup>26</sup> which should exhibit a gap energy scale different from that observed in the specific heat.

#### V. SUMMARY

We have shown that in weakly noncentrosymmetric superconductors, the Pauli depairing effect is anisotropic in the momentum space, inducing the point-node-like structure of the quasiparticle excitation energy gap even in isotropic s-wave states. This effect is caused by the competition between the asymmetric SO interaction and the Zeeman magnetic field in the superconducting state, and yields unique low temperature behaviors of thermodynamic quantities quite different from those of conventional s-wave superconductors. Also, by using the quasiclassical method, we have demonstrated that the magnetic field dependence of the specific heat exhibits a multi-gap-like structure for sufficiently small SO interaction even when there is only a single gap. These effects are associated with the momentum-dependent spin orientation of Cooper pairs which characterizes parityviolation. Thus, our results reveal the unique aspects of parity-violated Cooper pairs inherent in weakly noncentrosymmetric systems. We have also discussed that our findings may be relevant to the recent experimental observations for  $Y_2C_3$ .

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### APPENDIX A: QUASIPARTICLE ENERGY

The single-electron energies of the Hamiltonian (2) with the Zeeman term  $-\sum_{k,\sigma\sigma'}\mu_B H_z \sigma^z_{\sigma\sigma'} c^{\dagger}_{k\sigma} c_{k\sigma'}$  are given by the solutions of the following eigenvalue equation:

$$\begin{vmatrix} \varepsilon_{k} - \mu_{B}H_{z} + \mathcal{L}_{0z} - x & 0 & \mathcal{L}_{0x} - i\mathcal{L}_{0y} & \Delta \\ 0 & -\varepsilon_{k} + \mu_{B}H_{z} + \mathcal{L}_{0z} - x & -\Delta^{*} & \mathcal{L}_{0x} + i\mathcal{L}_{0y} \\ \mathcal{L}_{0x} + i\mathcal{L}_{0y} & -\Delta & \varepsilon_{k} + \mu_{B}H_{z} - \mathcal{L}_{0z} - x & 0 \\ \Delta^{*} & \mathcal{L}_{0x} - i\mathcal{L}_{0y} & 0 & -\varepsilon_{k} - \mu_{B}H_{z} - \mathcal{L}_{0z} - x \end{vmatrix} = 0.$$
(A1)

Here, the matrix is defined in the space spanned by the basis  $(c_{k\uparrow}^{\dagger}, c_{-k\uparrow}, c_{k\downarrow}^{\dagger}, c_{-k\downarrow})$ . The explicit solutions of Eq. (A1) are

$$E_{k1} = \frac{1}{2} \left( \sqrt{\tilde{\alpha}_{+}^{1/3} + \tilde{\alpha}_{-}^{1/3} - \frac{2}{3}X} + \sqrt{\frac{-2Y}{\sqrt{\tilde{\alpha}_{+}^{1/3} + \tilde{\alpha}_{-}^{1/3} - \frac{2}{3}X}} - \tilde{\alpha}_{+}^{1/3} - \tilde{\alpha}_{-}^{1/3} - \frac{4}{3}X} \right), \tag{A2}$$

$$E_{k2} = \frac{1}{2} \left( -\sqrt{\tilde{\alpha}_{+}^{1/3} + \tilde{\alpha}_{-}^{1/3} - \frac{2}{3}X} - \sqrt{\frac{2Y}{\sqrt{\tilde{\alpha}_{+}^{1/3} + \tilde{\alpha}_{-}^{1/3} - \frac{2}{3}X} - \tilde{\alpha}_{+}^{1/3} - \tilde{\alpha}_{-}^{1/3} - \frac{4}{3}X}} \right),$$
(A3)

$$E_{k3} = \frac{1}{2} \left( \sqrt{\tilde{\alpha}_{+}^{1/3} + \tilde{\alpha}_{-}^{1/3} - \frac{2}{3}X} - \sqrt{\frac{-2Y}{\sqrt{\tilde{\alpha}_{+}^{1/3} + \tilde{\alpha}_{-}^{1/3} - \frac{2}{3}X}} - \tilde{\alpha}_{+}^{1/3} - \tilde{\alpha}_{-}^{1/3} - \frac{4}{3}X} \right),$$
(A4)

$$E_{k4} = \frac{1}{2} \left( -\sqrt{\tilde{\alpha}_{+}^{1/3} + \tilde{\alpha}_{-}^{1/3} - \frac{2}{3}X} + \sqrt{\frac{2Y}{\sqrt{\tilde{\alpha}_{+}^{1/3} + \tilde{\alpha}_{-}^{1/3} - \frac{2}{3}X}} - \tilde{\alpha}_{+}^{1/3} - \tilde{\alpha}_{-}^{1/3} - \frac{4}{3}X} \right),$$
(A5)

where  $\tilde{\alpha}_{\pm}^{1/3} = e^{\pm i(4/3)\pi} \alpha_{\pm}^{1/3}$  and

$$\begin{aligned} \alpha_{\pm} &= \frac{1}{2} \left[ \frac{1}{27} (2X^3 + 36XZ) - 4XZ + Y^2 \right] \\ &\pm \sqrt{\left( \frac{1}{27} (2X^3 + 36XZ) - 4XZ + Y^2 \right)^2 - \frac{4}{729} (12Z + X^2)^3} \right], \end{aligned}$$
(A6)

with

$$X = -2(\varepsilon_k^2 + \alpha^2 |\mathcal{L}_0(k)|^2 + \mu_B^2 H_z^2 + \Delta^2), \qquad (A7)$$

$$Y = 8\mu_B H_z \alpha \mathcal{L}_{0z} \varepsilon_k, \tag{A8}$$

$$Z = (\varepsilon_k^2 - \alpha^2 | \mathcal{L}_0(k) |^2 - \mu_B^2 H_z^2)^2 + \Delta^4 + 2\Delta^2 \varepsilon_k^2 - 4\mu_B^2 H_z^2 \alpha^2 \mathcal{L}_{0z}^2.$$
(A9)

Since there is a term linear in x in Eq. (A1) with the coefficient given by Eq. (A8) for  $H_z \neq 0$ , the particle-hole symmetry is broken by the Zeeman magnetic field.<sup>21,36</sup>

# APPENDIX B: SOLUTIONS FOR QUASICLASSICAL GREEN FUNCTIONS

In this appendix, we present the explicit solutions for the spatially averaged quasiclassical Green functions satisfying Eqs. (11) and (12), which are derived from the Eilenberger equations (7) combined with the normalization condition  $\hat{g}\cdot\hat{g}=1$ . Using the decoupling approximation for the spatial average,  $\langle g^{(\mu\nu)2}\rangle \approx \langle g^{(\mu\nu)}\rangle^2$ ,  $\langle g^{(\mu\nu)}f^{(\kappa\lambda)}\Delta\rangle \approx \langle g^{(\mu\nu)}\rangle \langle f^{(\kappa\lambda)}\Delta\rangle$ , etc., we obtain the expressions for  $\langle g^{(\mu\mu)}\rangle$ ,

$$\begin{split} \langle g^{(++)}(p) \rangle &= -i \operatorname{sgn} \varepsilon_n [1 - P(\widetilde{\varepsilon}_n^{(++)}) | s_+(\hat{k}) |^2 \{1 - r(p) \\ &- 2\alpha (|\mathcal{L}'| - |\mathcal{L}|) s_2(\hat{k}) [a(p) + b(p)r(p)] \}^2 \\ &+ 4\alpha^2 |\mathcal{L}'|^2 | s_+(\hat{k}) |^2 [a(p) + b(p)r(p)]^2 - P(\widetilde{\varepsilon}_n^{(--)}) \\ &\times \{ s_2(\hat{k}) [1 + r_2(-p)] + 2\alpha (|\mathcal{L}'| + |\mathcal{L}|) \\ &\times |s_+(\hat{k})|^2 [a(p) + b(p)r(p)] \}^2 ]^{-1/2}, \end{split}$$
(B1)  
$$\langle g^{(--)}(p) \rangle = -r(p) r_2(p) \langle g^{(++)}(p) \rangle, \end{aligned}$$
(B2)

where

$$a(p) = \frac{is_2(\hat{k})}{\tilde{D}} \{Y(1) - Y(3) + r_2(-p)[Y(2) - Y(3)]\},$$
(B3)

$$b(p) = -\frac{is_2(\hat{k})}{\tilde{D}} \{Y(1) - Y(4) + r_2(-p)[Y(2) - Y(4)]\},$$
(B4)

$$r_{2}(p) = \frac{1}{A_{+}} [A_{-} + 8\alpha^{3}(|\mathcal{L}'| - |\mathcal{L}|)(|\mathcal{L}|^{2} - |\mathcal{L}'|^{2}) \\ \times |s_{+}(\hat{k})|^{2} s_{2}(\hat{k}) c_{0}^{3} Y(1)],$$
(B5)

$$\begin{aligned} A_{\pm} &= Y(1) - 2\alpha(|\mathcal{L}'| - |\mathcal{L}|)s_{2}(\hat{k})c_{0}Y(1) - 4\alpha|\mathcal{L}|s_{2}(\hat{k})c_{0}Y(3) \\ &+ 4\alpha^{2}(|\mathcal{L}'| + |\mathcal{L}|)|s_{+}(\hat{k})|^{2}c_{0}^{2}[Y(4)|\mathcal{L}'| - Y(3)|\mathcal{L}|] \\ &\pm 8\alpha^{2}(|\mathcal{L}|^{2} - |\mathcal{L}'|^{2})c_{0}|s_{+}(\hat{k})|^{2}(c_{\pm}\{Y(1) \\ &- 2\alpha|\mathcal{L}|Y(3)c_{0}s_{2}(\hat{k}) - \alpha(|\mathcal{L}'| \\ &- |\mathcal{L}|)s_{2}(\hat{k})c_{0}Y(1)\} \pm \alpha c_{0}^{2}s_{2}(\hat{k})[Y(3)|\mathcal{L}| \mp Y(4)|\mathcal{L}'|]), \end{aligned}$$
(B6)

$$c_{+} = \frac{is_{2}(\hat{k})}{\tilde{D}} [Y(2) - Y(1) + Y(4) - Y(3)], \qquad (B7)$$

$$c_{-} = \frac{is_{2}(\hat{k})}{\tilde{D}} [Y(4) + Y(3) - 2Y(2)],$$
(B8)

$$c_0 = \frac{is_2(\hat{k})}{\tilde{D}} [Y(1) + Y(2) - 2Y(3)], \tag{B9}$$

$$r(p) = \frac{1}{2R} \left[ -S + \operatorname{sgn} \varepsilon_n \sqrt{S^2 - 4RQ} \right], \qquad (B10)$$

$$Q = Y(1) - 2\alpha (|\mathcal{L}'| - |\mathcal{L}|) s_2(\hat{k}) Y(1) a(p) - 2\alpha |\mathcal{L}'| Y(4) [1 + r_2(p)] s_2(\hat{k}) a(p) + a(p)^2 h(p),$$
(B11)

$$R = -Y(1) - 2\alpha (|\mathcal{L}'| - |\mathcal{L}|) s_2(\hat{k}) Y(1) b(p) + 2\alpha |\mathcal{L}'| Y(4) [1 + r_2(p)] s_2(\hat{k}) b(p) + b(p)^2 h(p),$$
(B12)

$$S = -2\alpha (|\mathcal{L}'| - |\mathcal{L}|)s_2(\hat{k})Y(1)[a(p) + b(p)]$$
  
+  $2\alpha |\mathcal{L}'|Y(4)[1 + r_2(p)]s_2(\hat{k})a(p)$   
-  $2\alpha |\mathcal{L}|Y(3)[1 + r_2(-p)]s_2(\hat{k})b(p) + 2a(p)b(p)h(p),$   
(B13)

with

$$h(p) = 4\alpha^{2}(|\mathcal{L}'| + |\mathcal{L}|)|s_{+}(\hat{k})|^{2}[Y(4)|\mathcal{L}'| - Y(3)|\mathcal{L}|].$$
(B14)

Here,  $p = (\hat{k}, \varepsilon_n)$ ,  $Y(1) \equiv Y(\hat{\varepsilon}_n^{(++)})$ ,  $Y(2) \equiv Y(\hat{\varepsilon}_n^{(-+)})$ ,  $Y(3) \equiv Y(\hat{\varepsilon}_n^{(--)})$ , and  $Y(4) \equiv Y(\hat{\varepsilon}_n^{(+-)})$ .

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Substituting the above expressions for  $\langle g^{(\mu\mu)} \rangle$  into Eq. (12), we obtain the off-diagonal components of the normal Green functions  $\langle g^{(+-)} \rangle$  and  $\langle g^{(-+)} \rangle$ .

Because of the existence of the Zeeman magnetic field, the particle-hole symmetry does not hold, i.e.,  $\langle g^{(\mu\nu)}(-p) \rangle \neq -\langle g^{(\mu\nu)}(p) \rangle$ . Instead, we have

$$\langle g^{(++)}(-p)\rangle = r(p)\langle g^{(++)}(p)\rangle, \tag{B15}$$

$$\langle g^{(--)}(-p) \rangle = \frac{r_2(-p)}{r(p)r_2(p)} \langle g^{(--)}(p) \rangle,$$
 (B16)

$$\langle g^{(+-)}(-p)\rangle = -\frac{|\mathcal{L}(\hat{k})|}{|\mathcal{L}(-\hat{k})|}\langle g^{(+-)}(p)\rangle, \qquad (B17)$$

$$\langle g^{(-+)}(-p)\rangle = -\frac{|\mathcal{L}(\hat{k})|}{|\mathcal{L}(-\hat{k})|}\langle g^{(-+)}(p)\rangle. \tag{B18}$$

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