

# Signature of superconducting states in cubic crystal without inversion symmetry

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The effects of the absence of inversion symmetry on superconducting states are investigated theoretically. In particular, we focus on the noncentrosymmetric compounds that have the cubic symmetry  $O$  like  $\text{Li}_2\text{Pt}_3\text{B}$ . An appropriate and isotropic spin-orbital interaction is added in the Hamiltonian, and it acts like a magnetic monopole in the momentum space. The consequent pairing wave function has an additional triplet component in the pseudospin space, and a Zeeman magnetic field  $\mathbf{B}$  can induce a collinear supercurrent  $\mathbf{J}$  with a coefficient  $\kappa(T)$ . The effects of anisotropy embedded in the cubic symmetry and the nodal superconducting gap function on  $\kappa(T)$  are also considered. From the macroscopic perspectives, the pair of mutually induced  $\mathbf{J}$  and magnetization  $\mathbf{M}$  can affect the distribution of magnetic field in such noncentrosymmetric superconductors, which is studied through solving the Maxwell equation in the Meissner geometry as well as the case of a single vortex line. In both cases, magnetic fields perpendicular to the external ones emerge as a signature of the broken symmetry.

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## I. INTRODUCTION

The family of fermion superfluid, which includes the classes of conventional superconductor, helium-3 superfluid, and cuprate superconductor, has been one of the most frontier subjects in condensed matter physics. According to the parity symmetry of their pairing wave function,<sup>1</sup> the above classes can be labeled as  $s$ -wave,  $p$ -wave, and  $d$ -wave superfluids, respectively, and each has distinct thermodynamic and transport properties. In a system without inversion symmetry, this classification is, however, invalid, and the system is expected to simultaneously possess the properties belonging to distinct classes. The symmetry of the pairing wave functions as well as the gap functions is the immediate question. Theoretical studies based on the addition of a spin-orbital interaction in the Hamiltonian predict the Cooper pair to be a mixed state of singlets and triplets in pseudospin space,<sup>2</sup> which can lead to a nonvanishing spin susceptibility at zero temperature.<sup>2-4</sup> Besides, the nodal gap structure has been investigated experimentally<sup>5-8</sup> on two typical superconducting compounds,  $\text{CePt}_3\text{Si}$  and  $\text{Li}_2\text{Pt}_3\text{B}$ ,<sup>9,10</sup> which have the point group symmetries of  $C_{4v}$  and  $O$ , respectively.

On the other hand, the spin-orbital interaction also provides a correlation between the electric and magnetic degrees of freedom within the Fermi sea, connecting with the magnetic properties of the superconducting state in a subtle way. For example, a net polarization of spins can be induced by a shift of momenta distribution or vice versa in the superconducting state.<sup>3,11,12</sup> In other words, the supercurrent and magnetization can be mutually induced. Therefore, the macroscopic distributions of current and magnetic field in the superconducting state can also be used to probe the effect of lacking inversion symmetry.<sup>13-16</sup> One should note that the form of spin-orbital interaction must vary with the background crystals of different point group symmetries. Consequently, the magnetic properties pertaining to superconducting  $\text{CePt}_3\text{Si}$  and  $\text{Li}_2\text{Pt}_3\text{B}$  are expected to be quite different. However, almost all the previous theoretical studies are based on the symmetry of  $C_{4v}$ , which allows the Rashba form of spin-orbital interaction.

In this paper, we focus on the magnetic properties pertaining to the compounds with crystal symmetry of  $O$ , such as  $\text{Li}_2\text{Pt}_3\text{B}$ . The starting point is to write down an appropriate spin-orbital interaction, which turns out to act like a magnetic monopole in momentum space in this case. For simplicity, we first consider the case of isotropic Fermi surface and pairing gap. The supercurrent  $\mathbf{J}$  is found to have a component parallel to the applied Zeeman magnetic field  $\mathbf{B}$ , and the proportional constant  $\kappa$  is obtained by the linear response theory. For macroscopic studies, we employ the Maxwell equation to investigate the distribution of magnetic field in the Meissner geometry and the case of a single vortex line. Lastly, we also consider the effects of anisotropy embedded in the cubic symmetry, which causes a power-law dependence of  $\kappa(T)$  for very low temperature due to the appearance of line nodes of superconducting gap functions.

## II. MICROSCOPIC DERIVATION OF SUPERCURRENT INDUCED BY A ZEEMAN FIELD

The goal of this section is to obtain an expression for the supercurrent induced by a Zeeman magnetic field in the bulk superconductor without inversion symmetry. We first consider the normal state. The lack of inversion symmetry is manifested itself by the spin-orbital interaction in the Hamiltonian  $H = \sum_{\mathbf{p}} (H_{\mathbf{p}})_{\alpha\beta} a_{\mathbf{p}\alpha}^\dagger a_{\mathbf{p}\beta}$ , in which the operator is given by

$$H_{\mathbf{p}} = \frac{p^2}{2m} - E_F - \vec{h}_{\mathbf{p}} \cdot \vec{\sigma}, \quad (1)$$

and  $a_{\mathbf{p}\alpha}$  are the second-quantized operators for the electron of momentum  $\mathbf{p}$  and spin polarization  $\alpha = \{\uparrow, \downarrow\}$  is along the  $z$  axis in the laboratory frame. For convenience, we write  $\xi_{\mathbf{p}} = p^2/2m - E_F$ . Note that the spin-orbital interaction is characterized by the parity-breaking inner product consisting of a parity odd  $\vec{h}_{\mathbf{p}} = -\vec{h}_{-\mathbf{p}}$  and the spin  $\vec{\sigma}$ , which is invariant under spatial inversion. It is convenient to work in the helicity basis (labeled by  $\uparrow\downarrow$ ) in which the operator  $\vec{h}_{\mathbf{p}} \cdot \vec{\sigma}$  is diagonal, that is,

$$\hat{h}_{\mathbf{p}} \cdot \vec{\sigma} |\mathbf{p} \uparrow \downarrow\rangle = \pm |\mathbf{p} \uparrow \downarrow\rangle. \quad (2)$$

The eigenvalues of  $H_{\mathbf{p}}$  are thus given by  $\epsilon_{\mathbf{p}}^{\pm} = \xi_{\mathbf{p}} \mp h_{\mathbf{p}}$  for positive  $\uparrow$  and negative  $\downarrow$  helicities. Hence, the degenerate spectrum is split into two branches  $\pm$  in the presence of the spin-orbital interaction. The transformation between the helicity basis  $\uparrow\downarrow$  and the laboratory frame basis  $\uparrow\downarrow$  is given by the unitary operator  $U_{\mathbf{p}} = \exp(-\frac{i}{2}\hat{\mathbf{k}} \cdot \vec{\sigma} \theta_{\mathbf{p}})$ , which rotates the  $z$  axis by an angle of  $\theta_{\mathbf{p}}$  around the axis of  $\mathbf{k} = \mathbf{z} \times \hat{h}_{\mathbf{p}}$ . More explicitly, the matrix form of  $U_{\mathbf{p}}$  can be written down in terms of the coordinate of  $\hat{h}_{\mathbf{p}}$ , namely,

$$U_{\mathbf{p}} = \begin{pmatrix} \cos \frac{\theta_{\mathbf{p}}}{2} & -e^{-i\phi_{\mathbf{p}}} \sin \frac{\theta_{\mathbf{p}}}{2} \\ e^{i\phi_{\mathbf{p}}} \sin \frac{\theta_{\mathbf{p}}}{2} & \cos \frac{\theta_{\mathbf{p}}}{2} \end{pmatrix}. \quad (3)$$

Next, we include the pairing between two electrons of opposite momenta on the same branch. In the helicity basis, a general mean-field description for the pairing potential  $H_{\Delta}$  can be written as

$$H_{\Delta} = \sum_{\mathbf{p}} [\Delta_{+}^{*}(\mathbf{p}) a_{-\mathbf{p}\uparrow} a_{\mathbf{p}\uparrow} + \Delta_{-}^{*}(\mathbf{p}) a_{-\mathbf{p}\downarrow} a_{\mathbf{p}\downarrow} + \text{H.c.}], \quad (4)$$

where the two gap functions  $\Delta_{+}$  and  $\Delta_{-}$ , representing the pairing order parameter on the two branches, are not identical in general. However, the above pairing Hamiltonian can, by performing the transformation  $U$ , be restored to the case of a singlet whenever  $\Delta_{\pm}(\mathbf{p}) = e^{\mp i\phi_{\mathbf{p}}} |\Delta|$ . Now, the Nambu representation for the full Hamiltonian  $H$  in the helicity basis can be written as

$$H = \sum_{\mathbf{p}} (a_{\mathbf{p}\uparrow}^{\dagger} \ a_{-\mathbf{p}\uparrow}) \begin{pmatrix} \xi_{\mathbf{p}} - h_{\mathbf{p}} & \Delta_{+} \\ \Delta_{+}^{*} & -\xi_{\mathbf{p}} + h_{\mathbf{p}} \end{pmatrix} \begin{pmatrix} a_{\mathbf{p}\uparrow} \\ a_{-\mathbf{p}\uparrow}^{\dagger} \end{pmatrix} \\ + (a_{\mathbf{p}\downarrow}^{\dagger} \ a_{-\mathbf{p}\downarrow}) \begin{pmatrix} \xi_{\mathbf{p}} + h_{\mathbf{p}} & \Delta_{-} \\ \Delta_{-}^{*} & -\xi_{\mathbf{p}} - h_{\mathbf{p}} \end{pmatrix} \begin{pmatrix} a_{\mathbf{p}\downarrow} \\ a_{-\mathbf{p}\downarrow}^{\dagger} \end{pmatrix}. \quad (5)$$

In what follows, we employ the method of Matsubara Green's functions.<sup>17</sup> It is useful to introduce the Nambu spinor representations  $\Psi_{\mathbf{p}}$  and  $\tilde{\Psi}_{\mathbf{p}}$  for  $\uparrow\downarrow$  and  $\downarrow\uparrow$  bases, respectively,

$$\tilde{\Psi}_{\mathbf{p}} = \begin{pmatrix} a_{\mathbf{p}\uparrow} \\ a_{\mathbf{p}\downarrow} \\ a_{-\mathbf{p}\uparrow}^{\dagger} \\ a_{-\mathbf{p}\downarrow}^{\dagger} \end{pmatrix}, \quad \Psi_{\mathbf{p}} = \begin{pmatrix} a_{\mathbf{p}\uparrow} \\ a_{\mathbf{p}\downarrow} \\ a_{-\mathbf{p}\uparrow}^{\dagger} \\ a_{-\mathbf{p}\downarrow}^{\dagger} \end{pmatrix}. \quad (6)$$

The Matsubara Green's functions  $\check{G}$  in the  $\uparrow\downarrow$  basis are defined in a complex time-ordered manner as

$$G_{\alpha\beta}(\mathbf{p}, \tau) = -\langle T_{\tau} \Psi_{\mathbf{p}\alpha}(\tau) \Psi_{\mathbf{p}\beta}^{\dagger}(0) \rangle \quad (7)$$

and in the matrix form as

$$\check{G} = \begin{pmatrix} \hat{g} & \hat{f} \\ \hat{f} & \hat{f} \end{pmatrix}, \quad (8)$$

where  $\hat{g}$  and  $\hat{f}$  are the matrix forms of the ordinary Green's functions and Gor'kov Green's functions. We note that the lower components have the properties  $\hat{g}(\mathbf{p}, \tau) = -\hat{g}^{tr}(-\mathbf{p}, -\tau)$  and  $\hat{f}(\mathbf{p}, \tau) = \hat{f}^{\dagger}(\mathbf{p}, -\tau)$ . The Fourier transformation of  $G$  is given by

$$G_{\alpha\beta}(\mathbf{p}, \omega_n) = \frac{1}{\beta} \int_0^{\beta} d\tau e^{i\omega_n \tau} G_{\alpha\beta}(\mathbf{p}, \tau), \quad (9)$$

where  $1/\beta$  is the temperature and the frequency  $\omega_n = (2n+1)\pi/\beta$  is restricted due to the Fermi statistics. It is easier to first obtain the Green's function  $\check{G}$  by simply inverting the matrix  $(i\omega_n - H)$  in the helicity basis. The desired  $\check{G}$  can be obtained by performing the rotation in the pseudospin space using the following:

$$\hat{g}(\mathbf{p}) = U_{\mathbf{p}} \hat{g} U_{\mathbf{p}}^{\dagger}, \quad (10)$$

$$\hat{f}(\mathbf{p}) = U_{\mathbf{p}} \hat{f} U_{-\mathbf{p}}^{tr}, \quad (11)$$

where the transformation matrix  $U_{-\mathbf{p}}$  for the opposite momentum is given by  $U_{\mathbf{p}}(-i\sigma_y) e^{i\sigma_z \phi_{\mathbf{p}}}$ . Using the property that  $\sigma_y \vec{\sigma}^{tr} \sigma_y = -\vec{\sigma}$ , the expression for the Green's function  $\check{G}$  can be obtained as follows:

$$\hat{g} = \frac{1}{2} [(g_{+} + g_{-}) + (g_{+} - g_{-}) \hat{h}_{\mathbf{p}} \cdot \vec{\sigma}], \\ \hat{f} = \frac{1}{2} [(f_{+} + f_{-}) + (f_{+} - f_{-}) \hat{h}_{\mathbf{p}} \cdot \vec{\sigma}] (i\sigma_y), \quad (12)$$

where the scalar functions  $g_{\pm}$  and  $f_{\pm}$  are given below,

$$g_{\pm} = -\frac{i\omega_n + \epsilon_{\mathbf{p}}^{\pm}}{\omega_n^2 + \epsilon_{\mathbf{p}}^{\pm 2} + |\Delta_{\pm}|^2}, \\ f_{\pm} = \frac{\Delta_{\pm} e^{\pm i\phi_{\mathbf{p}}}}{\omega_n^2 + \epsilon_{\mathbf{p}}^{\pm 2} + |\Delta_{\pm}|^2}, \quad (13)$$

where we note that the previous condition for the pairing to recover the singlet is consistent with the condition for which the triplet component of Gor'kov Green's function vanishes in Eq. (12).

In what follows, we use the linear response theory to calculate the supercurrent  $\mathbf{J}$  induced by an external Zeeman magnetic field  $\vec{b}$ . We express the Fourier-transformed current operator in terms of the Nambu spinor representation as

$$\vec{J}_{\mathbf{q}} = \sum_{\mathbf{p}} \Psi_{\mathbf{p}-\alpha}^{\dagger}(\vec{v}_{\mathbf{p}})_{\alpha\beta} \Psi_{\mathbf{p}\beta}, \quad (14)$$

where the momentum  $\mathbf{p}_{\pm} = \mathbf{p} \pm \frac{\mathbf{q}}{2}$ , and the velocity operator  $\mathbf{v}_{\mathbf{p}}$  associated with momentum  $\mathbf{p}$  is obtained by taking the derivative of the Hamiltonian with respect to  $\mathbf{p}$ , which gives

an identical result with the previous studies,<sup>15</sup>

$$\check{v}_{\mathbf{p}} = \begin{pmatrix} \frac{\mathbf{p}}{m} - \nabla_{\mathbf{p}} \vec{h}_{\mathbf{p}} \cdot \vec{\sigma} & 0 \\ 0 & \frac{\mathbf{p}}{m} + \nabla_{\mathbf{p}} \vec{h}_{\mathbf{p}} \cdot \vec{\sigma}^{tr} \end{pmatrix}. \quad (15)$$

The paramagnetic perturbation  $V$  resulting from the Zeeman magnetic field  $\vec{b}(r)$  is  $V = -\mu \int dr \vec{s}(r) \cdot \vec{b}(r)$ ; here, the positive  $\mu$  is the magnetic moment and  $\vec{s}(r)$  denotes the local spin density.  $V$  can be represented in Fourier space as  $V = -\mu \vec{s}_{\mathbf{q}} \cdot \vec{b}_{-\mathbf{q}}$  in which the Fourier-transformed spin density is given by

$$\vec{s}_{\mathbf{q}} = \sum_{\mathbf{p}} \Psi_{\mathbf{p}-\mathbf{q}/2}^{\dagger} \vec{\Sigma} \Psi_{\mathbf{p}+\mathbf{q}/2}, \quad (16)$$

where  $\vec{\Sigma}$  is the spin operator for the Nambu spinor representation given by

$$\vec{\Sigma} = \begin{pmatrix} \vec{\sigma} & 0 \\ 0 & -\vec{\sigma}^{tr} \end{pmatrix}. \quad (17)$$

After some arrangement, the current  $\vec{J}$  can be written down explicitly as

$$\begin{aligned} \vec{J}(\mathbf{q}, i\omega_n) &= - \int_0^{\beta} d\tau e^{i\omega_n \tau} \langle T_{\tau} \vec{J}_{\mathbf{q}}^{\dagger}(\tau) \vec{s}_{\mathbf{q}}(0) \rangle \cdot (-\mu \vec{b}_{-\mathbf{q}}) \\ &= -\frac{\mu}{\beta} \sum_{\mathbf{p}} \sum_{\omega_m} \frac{1}{2} \text{Tr}' [\check{v}_{\mathbf{p}} \check{G}(\mathbf{p}_-, i\omega_m) (\vec{\Sigma} \cdot \vec{b}_{-\mathbf{q}}) \\ &\quad \times \check{G}(\mathbf{p}_+, i\omega_n + i\omega_m)], \end{aligned} \quad (18)$$

in which the symbol  $\text{Tr}'$  denotes taking trace over both the electron and hole sectors, and a factor of  $\frac{1}{2}$  is added to avoid double counting.

### III. MANIFESTATION OF THE ABSENCE OF INVERSION SYMMETRY

In this section, we are going to demonstrate the manifestation of the absence of inversion symmetry in this cubic superconductors from both microscopic and macroscopic perspectives. Starting from the general expression for supercurrent in Eq. (18), we investigate the static and homogeneous case; that is, the limits  $\mathbf{q} \rightarrow 0$  and  $\omega_n \rightarrow 0$  are taken. The resultant static current  $\mathbf{J}$  is collinear with the applied field, which can be written as

$$\mathbf{J} = -\kappa(T)\mathbf{B}, \quad (19)$$

where the macroscopic magnetic field or the magnetic induction is  $\mathbf{B} = \vec{b}_0$ . The appearance of this coefficient  $\kappa$  is an important signature of the lack of inversion symmetry. In Sec. III A,  $\kappa$  is studied explicitly for a given isotropic  $\vec{h}_{\mathbf{p}}$ .

Section III B is devoted to the studies of macroscopic aspects, which deals with the interaction between the magnetic field and the nonvanishing pairing order parameter  $\Delta$ . A crucial addition of Eq. (19) to the ordinary supercurrent and

the corresponding magnetization are the key ingredients for understanding the new distribution of magnetic field. By the way, the expressions for  $\mathbf{J}$  and  $\mathbf{M}$  can be obtained by taking the derivatives of free energy as<sup>14</sup>

$$\begin{aligned} \mathbf{J} &= 2 \frac{\delta F}{\delta \vec{q}}, \\ \mathbf{M} &= -\frac{\delta F}{\delta \mathbf{B}}, \end{aligned} \quad (20)$$

where the gauge-invariant phase gradient  $\vec{q} = \hbar \nabla \varphi + \frac{2e}{c} \mathbf{A}$  and the free energy  $F$  contains an extra term of  $-\frac{1}{2} \kappa \vec{q} \cdot \mathbf{B}$  representing the absence of inversion symmetry.<sup>14</sup> More explicitly, the above expressions can be written as

$$\frac{4\pi}{c} e \mathbf{J} = \frac{1}{\lambda^2} \left( \mathbf{A} + \frac{c\hbar}{2e} \nabla \varphi \right) - \frac{\delta}{\lambda^2} \mathbf{B}, \quad (21)$$

$$4\pi \mathbf{M} = \frac{\delta}{\lambda^2} \left( \mathbf{A} + \frac{c\hbar}{2e} \nabla \varphi \right). \quad (22)$$

$\lambda$  denotes the London penetration length. The length parameter  $\delta = \frac{4e\pi}{c} \kappa \lambda^2$  is introduced for later convenience. Note that we have taken the electronic charge to be  $(-e)$ .

#### A. Microscopic aspects

Now, we consider the simplest case for which the spin-orbital interaction is isotropic, and the gaps are identical for both branches and isotropic as well, that is,

$$\vec{h}_{\mathbf{p}} = \alpha \mathbf{p},$$

$$\Delta_+ = \Delta_- = \Delta. \quad (23)$$

The strength of the spin-orbital interaction is characterized by the quantity  $\alpha$ , which has the dimension of velocity and is weak in the sense that  $\alpha/v_F \ll 1$ . Here,  $v_F$  denotes the Fermi velocity. Starting from Eq. (18), with some arrangements, the static current can be obtained by taking the limit  $\mathbf{q} \rightarrow 0$  of the following expression:

$$\begin{aligned} \mathbf{J}_{\mathbf{q}} &= -\frac{\mu}{\beta} \int_{-\infty}^{+\infty} d\xi \nu(\xi) \\ &\quad \times \sum_{\omega_n} \sum_{\mu, \nu = \pm} Q_{\mu\nu} \frac{(i\omega_n + \epsilon_{\mathbf{p}_+}^{\mu})(i\omega_n + \epsilon_{\mathbf{p}_-}^{\nu}) + \Delta^2}{(\omega_n^2 + \epsilon_{\mathbf{p}_+}^{\mu 2} + \Delta^2)(\omega_n^2 + \epsilon_{\mathbf{p}_-}^{\nu 2} + \Delta^2)}, \end{aligned} \quad (24)$$

where the matrix elements of  $Q$  represent the factors for intrabranched contributions,  $\mu = \nu = \pm$ , and the interbranch ones,  $\mu = -\nu$ . Explicitly,  $Q$  in the matrix form can be written as

$$Q = \begin{pmatrix} \frac{1}{2}\vec{n} - \frac{1}{4}(\vec{l} + \vec{i}) & -\frac{1}{4}(\vec{l} - \vec{i}) \\ -\frac{1}{4}(\vec{l} - \vec{i}) & -\frac{1}{2}\vec{n} - \frac{1}{4}(\vec{l} + \vec{i}) \end{pmatrix}, \quad (25)$$

where the three vectors are obtained after the operation of trace and solid-angle integration, namely,

$$\begin{aligned} \vec{n} &= \int \frac{d\Omega}{4\pi} \text{Tr} \left[ \frac{\mathbf{p}}{m} (\vec{\sigma} \cdot \mathbf{B}) (\hat{\mathbf{p}} \cdot \vec{\sigma}) \right] = \frac{2}{3} \frac{p}{m} \mathbf{B}, \\ \vec{l} &= \int \frac{d\Omega}{4\pi} \text{Tr} [\alpha \vec{\sigma} (\vec{\sigma} \cdot \mathbf{B})] = 2\alpha \mathbf{B}, \\ \vec{i} &= \int \frac{d\Omega}{4\pi} \text{Tr} [\alpha \vec{\sigma} (\hat{\mathbf{p}} \cdot \vec{\sigma}) (\vec{\sigma} \cdot \mathbf{B}) (\hat{\mathbf{p}} \cdot \vec{\sigma})] = -\frac{2}{3} \alpha \mathbf{B}. \end{aligned} \quad (26)$$

Note that the trace here is only taken over a two-by-two helicity space in contrast to the previous operation in Eq. (18). First, we note that the static current in Eq. (24) is zero when the spin-orbital interaction is absent. For  $\vec{n}$ ,  $\vec{l}$ , and  $\vec{i}$  in Eq. (26), therefore, only the contributions up to first order  $\alpha/v_F$  are relevant. Since the summation over  $\omega_n$  will give a singular integrand concentrated at the Fermi level, it is eligible to substitute the quantities  $p$  and  $\nu(\xi)$  with their values at the Fermi level and then move them out of the integral. However, the contributions from  $\vec{n}$  in the diagonal parts of  $Q$  must be taken care of because explicitly they are of zeroth order of  $\alpha/v_F$ . Hence, the implicit contributions from the modification of the Fermi momentum and density of states due to the spin-orbital interaction have to be taken into account. Namely, the Fermi momentum for each branch,  $p_F^\pm = p_F(1 \pm \alpha/v_F)$ , and also the density of states at the Fermi level,  $\nu^\pm = m p_F^\pm (1 \pm \alpha/v_F)$ , should be used here. We also use the trick that enables performing the integration of energy first,<sup>18</sup> and after some algebra the coefficient  $\kappa$  is obtained as

$$\begin{aligned} \frac{\kappa(T)}{\mu\alpha\nu(0)} &= -\frac{4}{3} \left\{ \left[ 1 - \frac{\pi}{\beta} \sum_n \frac{\Delta^2}{(\omega_n^2 + \Delta^2)^{3/2}} \right] \right. \\ &\quad \left. - \left[ 1 - \frac{\pi}{\beta} \sum_n \frac{1}{(\omega_n^2 + \Delta^2)^{1/2}} \frac{\Delta^2}{\omega_n^2 + \Delta^2 + (\alpha p_F)^2} \right] \right\}. \end{aligned} \quad (27)$$

The term in the first bracket is actually the Yoshida function  $Y(\Delta, T)$ , which is a universal function characterizing the single-particle excitation across the gap  $\Delta$  at temperature  $T$ . For an isotropic gap and at low temperature  $T/\Delta \ll 1$ , the function  $Y$  is proportional to  $\exp(-\Delta/T)$ . The second bracket is identical to the first one when the spin-orbital interaction is absent. We denote this term by a function  $y(\Delta, \alpha, T)$  to represent the excitations between two superconducting states separated by an energy of  $\alpha p_F$ . Thus, we can rewrite Eq. (27) as  $\kappa = \frac{4}{3} \mu\alpha\nu(0)(y - Y)$ . At zero temperature, the function  $y$  can be evaluated by replacing the summation over the Matsubara frequency by an integral, and for isotropic  $\Delta$  and  $\alpha$ , this function is given by

$$y(\Delta, \alpha, T=0) = 1 - \frac{1}{2\theta} \frac{1}{\sqrt{1+\theta^2}} \ln(1 + 2\theta^2 + 2\theta\sqrt{1+\theta^2}), \quad (28)$$

where the number  $\theta = \alpha p_F/\Delta$ . For small  $\theta$ , the function  $y \sim \frac{2}{3}\theta^2$ . For large  $\theta$ , it is approximately  $1 - \frac{\ln(2\theta)}{\theta^2}$ . Both limits coincide with the previous predictions.<sup>2,12</sup>

In addition, the intrabranched and interbranched contributions can be respectively recognized as the Pauli and Van Vleck ones in the previous studies.<sup>12</sup> Therefore, the induced current  $\mathbf{J}$  is absent as the Pauli and Van Vleck contributions cancel each other in the normal state in which  $Y=y=1$ . On the other hand, the existence of such current relies on the fact that the Pauli paramagnetic contribution in the superconducting state is significantly suppressed, while the Van Vleck one is only reduced by a small portion as long as  $\Delta \ll \alpha p_F$ . Consequently, one can easily infer that the net supercurrent always flows opposite to the Pauli paramagnetic current.

## B. Macroscopic aspects

Here, the effect of lacking inversion symmetry on a macroscopic length scale is studied through solving the static Maxwell equation,

$$\nabla \times \mathbf{B} = 4\pi \nabla \times \mathbf{M} + \frac{4\pi}{c} (-e) \mathbf{J}. \quad (29)$$

Together with the current and magnetization given by Eqs. (21) and (22), we are able to obtain an equation in terms of the magnetic field  $\mathbf{B}$  only, namely,

$$\nabla \times \nabla \times \mathbf{B} = -\frac{1}{\lambda^2} \mathbf{B} + 2 \frac{\delta}{\lambda^2} \nabla \times \mathbf{B}, \quad (30)$$

in which the last curl term is generated from  $\nabla \times \mathbf{M}$  as well as the collinear supercurrent induced by  $\mathbf{B}$ . Hence, one can expect to observe a transverse component of the applied Zeeman field in such noncentrosymmetric superconductors.

Equation (30) can be applied for studying the penetration of the magnetic field in Meissner geometry. Explicitly, we can consider a cubic superconductor occupying the space for  $z > 0$ . It is convenient to first consider a general field  $B_x(z)\hat{x} + B_y(z)\hat{y}$  containing both  $x$  and  $y$  components. Consequently, the equation with which the general field satisfies is

$$\frac{d^2}{dz^2} B_+(z) = \frac{1}{\lambda^2} B_+(z) - 2i \frac{\delta}{\lambda^2} \frac{d}{dz} B_+(z), \quad (31)$$

where  $B_+$  stands for the linear combination  $B_x + iB_y$ . Defining  $B_+(z=0^+) = B_{\text{in},+}$ , the field just inside the superconductor, the general solution is then given by

$$B_+(z > 0) = B_{\text{in},+} e^{-z/\lambda(\sqrt{1-\delta^2/\lambda^2} + i(\delta/\lambda))}, \quad (32)$$

which is identical to the previous results.<sup>13</sup> So, one can expect a slight increase of penetration depth by a factor of  $1/\sqrt{1-\frac{\delta^2}{\lambda^2}}$  for such cubic superconductors in Meissner geometry. Besides, we note that the additional oscillation is a consequence of a parallel component of  $\mathbf{J}$  to  $\mathbf{B}$ .

The unknown  $B_{\text{in},+}$  in Eq. (32) can be determined from the boundary condition  $\mathbf{B}_{\text{ext}} = \mathbf{B}_{\text{in}} - 4\pi\mathbf{M}(z=0^+)$ , which requires the knowledge of magnetization  $\mathbf{M}$  or, equivalently, the gauge-invariant  $\vec{q}$ . In fact,  $\vec{q}$  can be obtained from the integration of the relation  $(-i)B_+(z) = dA_+(z)/dz$  with a given boundary condition at infinity. We can assume the homogeneity for phase  $\varphi$  throughout the superconductor, which is indicative of vanishing  $\mathbf{A}$  at  $z=\infty$  to ensure zero current there. Consequently, the boundary condition at the surface can be shown to, up to first order of  $\delta/\lambda$ , have the following form:

$$i\lambda B_{\text{ext},+} = A_{\text{in},+}. \quad (33)$$

A similar relation for  $B_-$  can be obtained from the above by taking complex conjugates on both sides.

If the external field is  $\mathbf{B}_{\text{ext}} = B\hat{x}$ , then  $A_x(0^+) = 0$  as a result of Eq. (33). Consequently,  $M_x(0^+) = 0$ , which demonstrates that the parallel field is continuous across the surface. In fact, the magnetic fields  $B_x$  and  $B_y$  inside the superconductor can be obtained by taking the real and imaginary parts of Eq. (32), respectively. Up to first order of  $\delta/\lambda$ , the two components can be written as

$$B_x = B \left[ \cos \frac{\delta z}{\lambda^2} + \frac{\delta}{\lambda} \sin \frac{\delta z}{\lambda^2} \right] e^{-z/\lambda}, \quad (34)$$

$$B_y = B \left[ \frac{\delta}{\lambda} \cos \frac{\delta z}{\lambda^2} - \sin \frac{\delta z}{\lambda^2} \right] e^{-z/\lambda}. \quad (35)$$

Along the direction of the applied field, the field  $B_x$  penetrates into the superconductor with an additionally slow oscillation of period about  $\lambda/\frac{\delta}{\lambda}$ . On the other hand,  $M_y(0^+)$  is finite due to the existence of finite flow velocity proportional to  $A_y$  at the interface. Hence, a discontinuity for field  $B_y$  is generated at the interface,

$$\frac{B_{\text{in},y} - B_{\text{ext},y}}{B_{\text{ext},x}} = \frac{\delta}{\lambda}, \quad (36)$$

which is different from the previous prediction for inversion-broken superconductor of the  $C_{4v}$  symmetry where the discontinuity happens to the parallel field across the interface.<sup>14</sup> The functional form of  $B_y$  in Eq. (35) indicates that it has the largest magnitude  $\frac{\delta}{\lambda}B$  at the surface, changes sign at  $z \cong \lambda$ , and then decays to zero while slowly oscillating. Furthermore, the flux associated with the perpendicular  $B_y$  is zero. This is consistent with the conclusion drawn from Eq. (33) that  $A_x = 0$  at the interface since both  $A_x(z=\infty)$  and  $A_z$  are zero.

Equation (30) can also be applied for studying a single vortex line as a macroscopic signature of lacking inversion symmetry. We consider the conventional case in which the vortex line is along the  $z$  axis, and the cylindrical coordinates are adopted here. The components of the magnetic field are assumed to be  $B_\phi(r)$  and  $B_z(r)$  along the directions of  $\hat{\phi}$  and  $\hat{z}$ , respectively. The  $z$  and  $\phi$  components of Eq. (30) are given by

$$\left[ \frac{1}{r} \frac{d}{dr} \left( r \frac{d}{dr} \right) - \frac{1}{\lambda^2} \right] B_z(r) = -\tilde{\kappa} \frac{1}{\lambda} \frac{d}{dr} (r B_\phi), \quad (37)$$

$$\left[ \frac{d}{dr} \left( \frac{1}{r} \frac{d}{dr} r \right) - \frac{1}{\lambda^2} \right] B_\phi(r) = \tilde{\kappa} \frac{1}{\lambda} \frac{d}{dr} B_z, \quad (38)$$

where we denote the dimensionless number  $\tilde{\kappa} = 2\delta/\lambda$  for convenience. We can therefore assume the following perturbation solutions:

$$B_z = B_z^{(0)} + \tilde{\kappa}^2 B_z^{(2)} + \dots, \quad (39)$$

$$B_\phi = \tilde{\kappa} B_\phi^{(1)} + \tilde{\kappa}^3 B_\phi^{(3)} + \dots. \quad (40)$$

The zeroth order solution  $B_z^{(0)}$  of Eq. (37) is just the conventional single vortex line solution, given by  $\frac{\Phi}{2\pi\lambda^2} K_0(r/\lambda)$ , where  $\Phi$  is a quantum of flux  $\frac{\pi\hbar c}{e}$  and  $K_0$  is the modified Bessel function of zeroth order. As can be seen in Eq. (38), now the transverse field  $B_\phi$  emerges as a result of the non-zero source proportional to  $K_1$  from the identity  $K'_0 = -K_1$ . Up to the first order of  $\tilde{\kappa}$ , the transverse field can be written down in terms of the Green's function  $g_1$  associated with Eq. (38).<sup>19</sup> Defining the dimensionless variable  $x$  as  $r/\lambda$ , it can be expressed as

$$\begin{aligned} B_\phi^{(1)}(x) / \frac{\Phi}{2\pi\lambda^2} &= \int_0^\infty x' dx' g_1(x, x') K_1(x') \\ &= K_1(x) \int_0^x x' dx' I_1(x') K_1(x') \\ &\quad + I_1(x) \int_x^\infty x' dx' [K_1(x')]^2, \end{aligned} \quad (41)$$

in which  $K_1$  and  $I_1$  are the modified Bessel functions of first order. The asymptotic behaviors of the transverse field distribution are

$$B_\phi^{(1)}(x) \sim \begin{cases} \frac{x}{2} \ln \frac{1}{x}, & x \rightarrow 0 \\ \sqrt{\frac{\pi x}{8}} e^{-x}, & x \rightarrow \infty \end{cases}. \quad (42)$$

Hence, the transverse field increases from zero at the origin, reaches its maximum at a distance of order  $\lambda$  from the center, and is followed by an exponential decay. The above extra magnetic fields noncollinear with the externally applied one can, in principle, be detected by observing the extra precession of polarized muons when their polarization is parallel to the external applied field.  $\frac{\delta}{\lambda}$  for  $\text{Li}_2\text{Pt}_3\text{B}$  is of order  $10^{-3}$  using the spin-orbital splitting estimated by Lee and Pickett.<sup>20</sup>

#### IV. ANISOTROPIC FERMI SURFACE AND LINE NODES OF GAP

In previous sections, we demonstrate an induced supercurrent parallel to the external Zeeman field as a signature of lacking inversion symmetry in cubic superconductors. Actually, the spin-orbital interaction appropriate for the point

group  $O$  respects all but the elements connected to inversion in  $O_h$ . The odd-parity basis functions<sup>21</sup>  $\{p_x^n \hat{x} + p_y^n \hat{y} + p_z^n \hat{z}; n = 1, 3, 5\}$ , in which the cubic symmetry is embedded, belonging to the  $A_{1u}$  representation within  $O_h$  can still be used to construct the vectors  $\vec{h}_p$ . Similarly, the general gap function respecting the cubic symmetry,

$$\hat{\Delta}(\mathbf{p}) = [\Delta_0(\mathbf{p}) + \vec{d}_p \cdot \vec{\sigma}](i\sigma_y), \quad (43)$$

can have the component  $\Delta_0(\mathbf{p})$  constructed from the even-parity basis functions belonging to the  $A_{1g}$  representation while the vector function  $\vec{d}_p$ , having identical symmetry properties of  $\vec{h}_p$ , can be constructed from the  $A_{1u}$  representation. Here, both components can be nonzero since parity is no longer respected. An important feature of the gap function given in Eq. (43) is the possible appearance of zeros when the order parameters  $\Delta_0(\mathbf{p})$  and  $\vec{d}_p$  can simultaneously be real after appropriate gauge transformations, which is true if the time-reversal symmetry is respected in the system. Consequently, it is possible to realize the zeros of the gap function when  $|\vec{d}_p|$  exceeds  $|\Delta_0(\mathbf{p})|$  for some points on the Fermi surface. Gapless excitation can therefore exist in such superconductors by showing, for example, a power law temperature dependence of penetration depth.<sup>22</sup>

In fact, the nodal structure of gap function in the compound  $\text{Li}_2\text{Pt}_3\text{B}$  was shown to be line nodes through the observation of linear temperature dependence in penetration depth for very low temperature.<sup>7,22</sup> Here, we shall investigate the effects of anisotropy and line nodes on the coefficient  $\kappa(T)$  near zero temperature. Since we are only interested in the regime of very weak Zeeman field, the anisotropy, which could result in some nonlinear field dependence for stronger field regime, has little qualitative effect here. Hence, only the line nodes of gap function are relevant to the low temperature behavior of  $\kappa(T)$ . The intrabranched, or the Pauli, contributions of  $\kappa(T)$  in Eq. (27) for the isotropic case can be generalized here by directly replacing the gaps  $\Delta_{\pm}$  with  $|\Delta_0| \pm |\vec{d}|$ . As for the interbranch contribution, the gaps on both branches are, in fact, much smaller than the separation  $\alpha p_F$  in  $\text{Li}_2\text{Pt}_3\text{B}$ , which suggests little relevance of actual gap function to this contribution. Moreover, even the appearance of zeros associated with the spin-orbital interaction,  $\alpha(\Omega)$  are also irrelevant to the  $T$  dependence of this contribution at very low temperature as long as the zeros associated with  $\alpha$  are not identical to those associated with the pairing gap.

We thus define a dimensionless quantity  $\gamma(T) \equiv \frac{\kappa(0) - \kappa(T)}{\kappa(0)}$  to present the temperature dependence due to the line nodes at temperature close to zero. Furthermore, from previous arguments, only the intrabranched contributions associated with the pairing gap of  $|\Delta_0| - |\vec{d}|$  is significant here. In addition, we are only interested in the effects due to the line nodes and take these parameters  $\alpha(\Omega)$  and  $v_F(\Omega)$  to be isotropic, which makes the evaluation easier and more accessible. Next, the summation over  $\omega_n$  in the function  $Y$  in Eq. (27) can be transformed into an integral of energy, which makes  $\gamma(T)$  into the following form:

$$\gamma(T) = \int \frac{d\Omega}{4\pi} (\cos \theta)^2 \Delta_-^2(\hat{\Omega}) \int_0^{\infty} d\xi \left( \frac{1}{E^3} \frac{2}{e^{\xi/T} + 1} + \frac{1}{2E^2 T \cosh^2(E/2T)} \right), \quad (44)$$

where the Zeeman field is assumed to be along the  $z$  axis, and  $\Delta_-(\hat{\Omega})$  denotes the gap functions of the direction  $\hat{\Omega}$  on the Fermi surface, and  $E = \sqrt{\xi^2 + \Delta_-^2(\hat{\Omega})}$ . We note that the above integral vanishes when  $T$  is exactly zero since  $E$  is always positive for all  $\xi$ . Hence, the contribution for  $T$  slightly larger than zero comes from integration around the solid angles  $\Omega$  associated with the zeros of gap. By the cubic symmetry, we can infer that there are six sets of line nodes on the Fermi surface, which as a whole remain invariant under any cubic rotation. Hence, the contributions from the six sets can be divided into  $\gamma(T) = 2\gamma_{\parallel}(T) + 4\gamma_{\perp}(T)$ , where  $\gamma_{\parallel}$  denotes that from the line nodes that are symmetrically distributed around the  $z$  axis, while  $\gamma_{\perp}$  denotes remaining sets that are around the  $x$  or  $y$  axis.

For a given set of line nodes, the gap function can be expanded around these zeros in the following manner:

$$\Delta_-(\hat{\Omega}) = \Delta'(\theta_c)(\theta - \theta_c), \quad (45)$$

which means that the solid angle  $\hat{\Omega} = (\theta, \phi)$  associated with the zeros can be parametrized as  $[\theta_c(\phi), \phi]$  along the azimuthal direction.  $\Delta'(\theta_c)$  denotes the slope of gap function along the direction of  $\hat{\theta}$ . Finally, the linear temperature dependence can be extracted from  $\gamma(T)$ , and the following expression can be obtained if one extends the upper limit of  $\theta$  integral to infinity:

$$\begin{aligned} & \begin{pmatrix} \gamma_{\parallel}(T) \\ \gamma_{\perp}(T) \end{pmatrix} \\ &= \int \frac{d\phi}{2\pi} \begin{pmatrix} \cos^2 \theta_c \\ \sin^2 \theta_c \cos^2 \phi \end{pmatrix} \frac{T}{\Delta'(\theta_c)} \\ & \quad \times \int_0^{\infty} \int_0^{\infty} x^2 dx dy \left( \frac{2}{r^3} \frac{1}{e^r + 1} + \frac{1}{2r^2} \frac{1}{\cosh^2(r/2)} \right), \end{aligned} \quad (46)$$

in which  $x = \theta \Delta'(\theta_c)/T$ ,  $y = \xi/T$ , and  $r = \sqrt{x^2 + y^2}$ . In terms of polar coordinate, the integral is to give  $\pi \ln 2$ .

## V. CONCLUSIONS

In this work, we demonstrate an induced supercurrent parallel to the external Zeeman magnetic field utilizing the Green's function method. Besides, the induced supercurrent

and the consequent magnetization modify the distribution of magnetic fields in the Meissner geometry as well as in the vortex line. Transverse magnetic fields are generated as a sign of breaking inversion symmetry in superconductors of point group symmetry  $O$  such as  $\text{Li}_2\text{Pt}_3\text{B}$ .

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