# Nonuniform states in noncentrosymmetric superconductors: Derivation of Lifshitz invariants from microscopic theory

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In noncentrosymmetric crystals, nonuniform superconducting states are possible even in the absence of any external magnetic field. The origin of these states can be traced to the Lifshitz invariants in the free energy, which are linear in spatial gradients. We show how various types of the Lifshitz invariants in noncentrosymmetric superconductors can be derived from microscopic theory.

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# I. INTRODUCTION

The discovery of superconductivity in CePt<sub>3</sub>Si (Ref. 1) has renewed interest, both experimental and theoretical, in the properties of superconductors without inversion symmetry. One of the most spectacular differences from the usual, i.e., centrosymmetric, case is the presence of additional terms in the Ginzburg-Landau free energy, which are linear in spatial gradients.<sup>2</sup> These terms lead to a "helical" superconducting phase, in which the order parameter is nonuniform in the presence of an external magnetic field which is coupled only to the spins of electrons.<sup>3,4</sup> That a nonuniform superconducting state can be created by purely paramagnetic effects was suggested a long time ago by Larkin and Ovchinnikov,<sup>5</sup> and Fulde and Ferrell<sup>6</sup> (LOFF). In contrast to the helical state, the LOFF state appears as a result of the sign change of the second-order gradient term in the free energy.

According to Refs. 7 and 8, the crystal symmetry might sometimes admit the linear in gradient terms—the Lifshitz invariants—in the free energy, leading to nonuniform superconducting states even in the absence of magnetic field. Our purpose here is to show how the Lifshitz invariants at zero field can be obtained microscopically in noncentrosymmetric superconductors with a Rashba-type spin-orbit (SO) coupling. In Sec. II, the case of a spin-triplet order parameter which transforms according to a three-dimensional irreducible representation of a cubic point group is discussed while in Sec. III we consider a mixture of two representations in a tetragonal crystal. The discussion of general situation is found in Sec. IV. Throughout the paper we use the units in which  $\hbar = k_B = 1$ , and *e* denotes the absolute value of the electron charge.

#### **II. INTERBAND PAIRING: SINGLE REPRESENTATION**

Our starting point is the following Hamiltonian of noninteracting electrons in a noncentrosymmetric crystal:

$$H_0 = \sum_{k} \sum_{\alpha\beta=\uparrow,\downarrow} \left[ \epsilon_0(k) \,\delta_{\alpha\beta} + \gamma(k) \,\boldsymbol{\sigma}_{\alpha\beta} \right] a_{k\alpha}^{\dagger} a_{k\beta}, \qquad (1)$$

where  $\sigma$  are the Pauli matrices and the sum over k is restricted to the first Brillouin zone. The second term in Eq. (1), with  $\gamma(k) = -\gamma(-k)$ , describes the Rashba-type (or antisymmetric) SO coupling of electrons with the crystal lattice,

which is specific to noncentrosymmetric systems. Equation (1) should be considered as a single-band effective Hamiltonian, in which  $\alpha$  and  $\beta$  are to be interpreted as pseudospin projections. The Hamiltonian is diagonalized by a unitary transformation  $a_{k\alpha} = \sum_{\lambda} u_{\alpha\lambda}(k) c_{k\lambda}$ , where

$$u_{\uparrow\lambda}(\boldsymbol{k}) = \sqrt{\frac{|\boldsymbol{\gamma}| + \lambda \gamma_z}{2|\boldsymbol{\gamma}|}}, \quad u_{\downarrow\lambda}(\boldsymbol{k}) = \lambda \frac{\gamma_x + i\gamma_y}{\sqrt{2|\boldsymbol{\gamma}|(|\boldsymbol{\gamma}| + \lambda \gamma_z)}}, \quad (2)$$

with the following result:

$$H_0 = \sum_{k} \sum_{\lambda = \pm} \xi_{\lambda}(k) c_{k\lambda}^{\dagger} c_{k\lambda}.$$
 (3)

Here the band dispersion functions are  $\xi_{\lambda}(k) = \epsilon_0(k) + \lambda |\gamma(k)|$ . The normal-state electron Green's functions can be written as

$$\hat{G}(\boldsymbol{k},\omega_n) = \sum_{\lambda=\pm} \hat{\Pi}_{\lambda}(\boldsymbol{k}) G_{\lambda}(\boldsymbol{k},\omega_n), \qquad (4)$$

where

$$\hat{\Pi}_{\lambda}(\boldsymbol{k}) = \frac{1 + \lambda \,\hat{\gamma}(\boldsymbol{k})\,\boldsymbol{\sigma}}{2} \tag{5}$$

are the band projection operators  $(\hat{\gamma} = \gamma / |\gamma|)$ , and

$$G_{\lambda}(\boldsymbol{k},\omega) = \frac{1}{i\omega_n - \xi_{\lambda}(\boldsymbol{k})}$$
(6)

are the Green's functions in the band representation.

In this section we show how one can obtain the Lifshitz invariants for an order parameter corresponding to a single irreducible representation of the crystal point group. Let us consider a purely triplet order parameter, which transforms according to an irreducible representation  $\Gamma$  (of dimensionality  $d_{\Gamma}$ ):

$$\mathbf{d}(\boldsymbol{k},\boldsymbol{r}) = \sum_{a=1}^{d_{\Gamma}} \eta_a(\boldsymbol{r})\varphi_a(\boldsymbol{k}), \tag{7}$$

where  $\varphi_a(k) = -\varphi_a(-k)$  are the spin-vector basis functions (see Ref. 9). The order-parameter matrix in the spin (or pseudospin) representation has the form  $\Delta_{\alpha\beta}(k,r) = d(k,r)g_{\alpha\beta}$ , where  $\hat{g} = i\hat{\sigma}\hat{\sigma}_2$ . Using the standard formalism (see, e.g., Ref. 10), we obtain for the quadratic terms in the free-energy density:

$$F_{2} = \frac{1}{V} \sum_{a} \eta_{a}^{*} \eta_{a} - \sum_{a,b} \eta_{a}^{*} \hat{K}_{ab} \eta_{b}, \qquad (8)$$

where V > 0 is the coupling constant, and the operator  $\hat{K}_{ab}$  is obtained from

$$K_{ab}(\boldsymbol{q}) = \frac{1}{2}T\sum_{n} \int \frac{d^{3}\boldsymbol{k}}{(2\pi)^{3}} \varphi_{a,i}^{*}(\boldsymbol{k})\varphi_{b,j}(\boldsymbol{k})$$
$$\times \operatorname{tr}[\hat{g}_{i}^{\dagger}\hat{G}(\boldsymbol{k}+\boldsymbol{q},\omega_{n})\hat{g}_{j}\hat{G}^{T}(-\boldsymbol{k},-\omega_{n})] \qquad (9)$$

by replacing  $q \rightarrow D = -i\nabla + (2e/c)A$ . The Matsubara summation is restricted by the cut-off energy  $\omega_c$ . Substituting here expression (4) and using the identity

$$\operatorname{tr}[\hat{g}_{i}^{\dagger}\hat{\Pi}_{\lambda_{1}}(\boldsymbol{k}+\boldsymbol{q})\hat{g}_{j}\hat{\Pi}_{\lambda_{2}}^{T}(-\boldsymbol{k})] = \frac{1-\lambda_{1}\lambda_{2}}{2}\delta_{ij} + \lambda_{1}\lambda_{2}\hat{\gamma}_{i}(\boldsymbol{k})\hat{\gamma}_{j}(\boldsymbol{k})$$
$$-\frac{i}{2}(\lambda_{1}-\lambda_{2})e_{ijl}\hat{\gamma}_{l}(\boldsymbol{k})$$

(here we neglected the corrections of the order of  $q/k_F$ ), we obtain

$$K_{ab}(\boldsymbol{q}) = \frac{1}{2}T\sum_{n}\sum_{\lambda}\int \frac{d^{3}\boldsymbol{k}}{(2\pi)^{3}}\varphi_{a,i}^{*}(\boldsymbol{k})\varphi_{b,j}(\boldsymbol{k})\{\hat{\gamma}_{i}(\boldsymbol{k})\,\hat{\gamma}_{j}(\boldsymbol{k})$$
$$\times G_{\lambda}(\boldsymbol{k}+\boldsymbol{q},\omega_{n})G_{\lambda}(-\boldsymbol{k},-\omega_{n}) + [\delta_{ij}-\hat{\gamma}_{i}(\boldsymbol{k})\,\hat{\gamma}_{j}(\boldsymbol{k})$$
$$-i\lambda e_{ijl}\hat{\gamma}_{l}(\boldsymbol{k})]G_{\lambda}(\boldsymbol{k}+\boldsymbol{q},\omega_{n})G_{-\lambda}(-\boldsymbol{k},-\omega_{n})\}.$$
(10)

The intergrand includes the intraband  $\propto G_{\lambda}G_{\lambda}$  as well as the interband  $\propto G_{\lambda}G_{-\lambda}$  pairing terms.

The Lifshitz invariants originate from the odd in q contribution to the kernel, which in turn comes from the last (linear in  $\hat{\gamma}$ ) term of Eq. (10):

$$K_{ab}^{L}(\boldsymbol{q}) = -\frac{i}{2} q_{m} e_{ijl} T \sum_{n} \sum_{\lambda} \lambda \int \frac{d^{3}\boldsymbol{k}}{(2\pi)^{3}} \varphi_{a,i}^{*}(\boldsymbol{k}) \varphi_{b,j}(\boldsymbol{k})$$
$$\times \hat{\gamma}_{l}(\boldsymbol{k}) v_{\lambda,m}(\boldsymbol{k}) G_{\lambda}^{2}(\boldsymbol{k},\omega_{n}) G_{-\lambda}(-\boldsymbol{k},-\omega_{n}).$$
(11)

Neglecting the difference (of the order of  $|\gamma|/\epsilon_F$ ) between the Fermi velocities in the two bands, i.e., setting  $v_+(k) = v_-(k) = v_F(k)$ , and calculating the Matsubara sums, we obtain in the vicinity of the critical temperature:

$$K_{ab}^{L}(\boldsymbol{q}) = -i\frac{N_{F}}{4\pi T_{c0}}q_{m}e_{ijl}\langle\Phi(\boldsymbol{k})\varphi_{a,i}^{*}(\boldsymbol{k})\varphi_{b,j}(\boldsymbol{k})\hat{\gamma}_{l}(\boldsymbol{k})\upsilon_{F,m}(\boldsymbol{k})\rangle_{\hat{\boldsymbol{k}}},$$
(12)

where the angular brackets denote the Fermi-surface averaging,

$$\Phi(\mathbf{k}) = \operatorname{Im} \Psi'\left(\frac{1}{2} + i\frac{|\boldsymbol{\gamma}(\mathbf{k})|}{2\pi T_{c0}}\right) \simeq -\frac{7\zeta(3)|\boldsymbol{\gamma}(\mathbf{k})|}{\pi T_{c0}},$$

and  $\Psi(x)$  is the digamma function. We assume that the Rashba SO coupling is sufficiently weak in order for the interband pairing to survive. We note that, in the absence of time-reversal symmetry breaking in the normal state, the ba-

sis functions can be chosen real. Then it follows from Eq. (12) that the Lifshitz invariants are absent for order parameters transforming according to one-dimensional representations of the point group.

Let us consider as an example a three-dimensional order parameter  $\eta = (\eta_1, \eta_2, \eta_3)$  in a cubic superconductor, which corresponds to the representation  $F_1$  of the point group G =**O**. We assume a spherical Fermi surface and describe the SO coupling by

$$\boldsymbol{\gamma}(\boldsymbol{k}) = \boldsymbol{\gamma}_0 \boldsymbol{k},\tag{13}$$

where  $\gamma_0$  is a constant. For the band dispersions we have  $\xi_{\lambda}(\mathbf{k}) = \epsilon_0(\mathbf{k}) + \lambda \alpha$ , where  $\alpha = |\gamma_0|k_F$  is the measure of the SO band splitting ( $k_F$  is the Fermi wave vector). The normalized spin-vector basis functions have the following form:

$$\varphi_{a,i}(\boldsymbol{k}) = \sqrt{\frac{3}{2}} e_{aij} \hat{k}_j. \tag{14}$$

Inserting this into Eq. (12), we obtain  $K_{ab}^L(q) = i(7\zeta(3)/8\pi^2)(N_F v_F \alpha/T_{c0}^2)e_{abi}q_i$ . From this it follows that the Lifshitz invariant in the free-energy density has the following form:

$$F_L = iK(\eta_1^* D_y \eta_3 + \eta_2^* D_z \eta_1 + \eta_3^* D_x \eta_2 - \text{c.c}), \qquad (15)$$

where

$$\tilde{K} = \frac{7\zeta(3)N_F v_F^2}{8\pi^2 T_{c0}^2} \frac{\alpha}{v_F}.$$
(16)

Note that, according to Eq. (14), the order parameter (7) satisfies  $d(k,r) \perp \gamma(k)$ . In the band representation, this corresponds to interband pairing, as opposed to the limit of strong SO band splitting, in which only the component  $d \parallel \gamma$  survives (intraband or "protected" component), in addition to the spin-singlet component.<sup>11</sup>

### III. INTERBAND PAIRING: MIXTURE OF TWO REPRESENTATIONS

In this section we discuss a different mechanism of producing the Lifshitz invariants. We start with the pairing interaction in the band representation, which can be written a general form as follows:

$$H_{\text{int}} = \frac{1}{2\mathcal{V}} \sum_{\boldsymbol{k}\boldsymbol{k}'\boldsymbol{q}} \sum_{\lambda_{1,2,3,4}} t_{\lambda_2}(\boldsymbol{k}) t^*_{\lambda_3}(\boldsymbol{k}') \widetilde{\mathcal{V}}_{\lambda_1 \lambda_2 \lambda_3 \lambda_4}(\boldsymbol{k}', \boldsymbol{k}') \\ \times c^{\dagger}_{\boldsymbol{k}+\boldsymbol{q},\lambda_1} c^{\dagger}_{-\boldsymbol{k},\lambda_2} c_{-\boldsymbol{k}',\lambda_3} c_{\boldsymbol{k}'+\boldsymbol{q},\lambda_4}, \qquad (17)$$

where

$$t_{\lambda}(\boldsymbol{k}) = \lambda \frac{\gamma_{x}(\boldsymbol{k}) - i\gamma_{y}(\boldsymbol{k})}{\sqrt{\gamma_{x}^{2}(\boldsymbol{k}) + \gamma_{y}^{2}(\boldsymbol{k})}}$$
(18)

are phase factors,

$$\widetilde{V}_{\lambda_1\lambda_2\lambda_3\lambda_4}(\boldsymbol{k},\boldsymbol{k}') = \upsilon_g(\boldsymbol{k},\boldsymbol{k}')\,\delta_{\lambda_1\lambda_2}\delta_{\lambda_3\lambda_4} + \upsilon_{u,ij}(\boldsymbol{k},\boldsymbol{k}')\,\tau_{i,\lambda_1\lambda_2}(\boldsymbol{k})\,\tau_{j,\lambda_3\lambda_4}(\boldsymbol{k}') + \upsilon_{m,i}(\boldsymbol{k},\boldsymbol{k}')\,\tau_{i,\lambda_1\lambda_2}(\boldsymbol{k})\,\delta_{\lambda_2\lambda_4}$$

$$+ v_{m,i}(\boldsymbol{k}',\boldsymbol{k}) \,\delta_{\lambda_1 \lambda_2} \tau_{i,\lambda_3 \lambda_4}(\boldsymbol{k}'), \qquad (19)$$

and  $\hat{\tau}_i(\mathbf{k}) = \hat{u}^{\dagger}(\mathbf{k}) \hat{\sigma}_i \hat{u}(\mathbf{k})$ , with the matrices  $\hat{u}(\mathbf{k})$  defined by Eq. (2). The functions  $v_g$ ,  $v_{u,ij}$ , and  $v_{m,i}$  describe the pairing strength and anisotropy in spin singlet, spin triplet, and mixed channels, respectively. We follow the notations of Ref. 12 and assume that the frequency dependence of the pairing amplitudes is factorized. The terms with  $\lambda_1 = \lambda_2$  and  $\lambda_3 = \lambda_4$  describe intraband pairing and the scattering of the Cooper pairs from one band to the other while the remaining terms describe pairing of electrons from different bands.

Treating the interaction (17) in the mean-field approximation, one introduces the gap functions  $\tilde{\Delta}_{\lambda_1\lambda_2}(k,q) = t^*_{\lambda_2}(k)\Delta_{\lambda_1\lambda_2}(k,q)$  with the following symmetry properties:

$$\widetilde{\Delta}_{\lambda_1\lambda_2}(\boldsymbol{k},\boldsymbol{q}) = \lambda_1\lambda_2\widetilde{\Delta}_{\lambda_2\lambda_1}(-\boldsymbol{k},\boldsymbol{q}).$$
<sup>(20)</sup>

These are related to the symmetry of the pairing interaction:  $\tilde{V}_{\lambda_2\lambda_1\lambda_3\lambda_4}(-\boldsymbol{k},\boldsymbol{k}') = \lambda_1\lambda_2\tilde{V}_{\lambda_1\lambda_2\lambda_3\lambda_4}(\boldsymbol{k},\boldsymbol{k}')$ , which can be easily established from Eq. (17). Near the critical temperature, the gap functions satisfy the linearized gap equations:

$$\widetilde{\Delta}_{\lambda_{1}\lambda_{2}}(\boldsymbol{k},\boldsymbol{q}) = -T\sum_{n} \int \frac{d^{3}\boldsymbol{k}'}{(2\pi)^{3}} \sum_{\lambda_{3}\lambda_{4}} \widetilde{V}_{\lambda_{1}\lambda_{2}\lambda_{4}\lambda_{3}}(\boldsymbol{k},\boldsymbol{k}')$$
$$\times G_{\lambda_{3}}(\boldsymbol{k}'+\boldsymbol{q},\omega_{n})G_{\lambda_{4}}(-\boldsymbol{k}',-\omega_{n})\widetilde{\Delta}_{\lambda_{3}\lambda_{4}}(\boldsymbol{k}',\boldsymbol{q}),$$
(21)

where  $G_{\lambda}(\mathbf{k}, \omega_n)$  are the Green's functions of band electrons [see Eq. (6)].

We describe pairing anisotropy by the following model, which is compatible with all symmetry requirements:

$$v_g(\mathbf{k}, \mathbf{k}') = -V_g,$$

$$v_{u,ij}(\mathbf{k}, \mathbf{k}') = -V_u(\hat{\boldsymbol{\gamma}}(\mathbf{k}) \hat{\boldsymbol{\gamma}}(\mathbf{k})) \delta_{ij},$$

$$v_{m,i}(\mathbf{k}, \mathbf{k}') = 0,$$
(22)

where  $V_g$  and  $V_u$  are constants. Then, from Eq. (19) one obtains

$$\widetilde{V}_{\lambda_{1}\lambda_{2}\lambda_{3}\lambda_{4}}(\boldsymbol{k},\boldsymbol{k}') = -V_{g}\delta_{\lambda_{1}\lambda_{2}}\delta_{\lambda_{3}\lambda_{4}} - V_{u}[\hat{\boldsymbol{\gamma}}(\boldsymbol{k})\,\hat{\boldsymbol{\gamma}}(\boldsymbol{k}')] \\ \times [\tau_{\lambda_{1}\lambda_{2}}(\boldsymbol{k})\,\tau_{\lambda_{2}\lambda_{4}}(\boldsymbol{k}')].$$
(23)

Further steps essentially depend on the crystal symmetry, which determines the momentum dependence of the SO coupling. Let us consider a tetragonal superconductor with the point group  $G = C_{4v}$ , in which case one can write

$$\boldsymbol{\gamma}(\boldsymbol{k}) = \boldsymbol{\gamma}_0(\hat{\boldsymbol{z}} \times \boldsymbol{k}), \qquad (24)$$

where  $\gamma_0$  is a constant. We assume a cylindrical Fermi surface along the *z* axis. For the band dispersions we then have  $\xi_{\lambda}(\mathbf{k}) = \epsilon_0(\mathbf{k}) + \lambda \alpha$ , where  $\alpha = |\gamma_0| k_F$ . From Eq. (23) we obtain the pairing interaction components as follows:

$$\begin{split} \widetilde{V}_{++++} &= \widetilde{V}_{----} = - V_g - V_u M^2, \\ \widetilde{V}_{++--} &= \widetilde{V}_{--++} = - V_g + V_u M^2, \end{split}$$

$$\begin{split} \widetilde{V}_{+-+-} &= \widetilde{V}_{-+++} = -V_{u}M + V_{u}M^{2}, \\ \widetilde{V}_{+--+} &= \widetilde{V}_{-++-} = -V_{u}M - V_{u}M^{2}, \\ \widetilde{V}_{+++-} &= \widetilde{V}_{+---} = \widetilde{V}_{-+++} = \widetilde{V}_{--+-} = iV_{u}MN, \\ \widetilde{V}_{++-+} &= \widetilde{V}_{+-++} = \widetilde{V}_{-+--} = \widetilde{V}_{-+--} = -iV_{u}MN, \end{split}$$
(25)

where  $M = \hat{k}\hat{k}'$  and  $N = (\hat{k} \times \hat{k}')_z$ . Note that the interband components in the third and the fourth lines here contain terms that are even in both k and k', as well as ones that are odd in k and k'. As we shall see, this gives rise to inhomogeneous superconducting states.

The pairing interaction can be presented as an expansion over the irreducible representations  $\Gamma$  of the point group G. The tetragonal group  $C_{4v}$  has four one-dimensional representations:  $A_1$ ,  $A_2$ ,  $B_1$ , and  $B_2$ , and one two-dimensional representation E (the notations are the same as in Ref. 13). The simplest polynomial expressions for the normalized basis functions have the following form:

$$\varphi_{A_1}(\mathbf{k}) = \hat{k}_x^2 + \hat{k}_y^2 = 1,$$
  

$$\varphi_{B_1}(\mathbf{k}) = \sqrt{2}(\hat{k}_x^2 - \hat{k}_y^2), \quad \varphi_{B_2}(\mathbf{k}) = 2\sqrt{2}\hat{k}_x\hat{k}_y,$$
  

$$\varphi_E(\mathbf{k}) = \sqrt{2}(\hat{k}_x, \hat{k}_y).$$
(26)

Using

$$M = \frac{1}{2}\varphi_{E}(\mathbf{k})\varphi_{E}(\mathbf{k}'),$$

$$M^{2} = \frac{1}{2}\varphi_{A_{1}}(\mathbf{k})\varphi_{A_{1}}(\mathbf{k}') + \frac{1}{4}\varphi_{B_{1}}(\mathbf{k})\varphi_{B_{1}}(\mathbf{k}') + \frac{1}{4}\varphi_{B_{2}}(\mathbf{k})\varphi_{B_{2}}(\mathbf{k}'),$$

$$MN = \frac{1}{4}\varphi_{B_{1}}(\mathbf{k})\varphi_{B_{2}}(\mathbf{k}') - \frac{1}{4}\varphi_{B_{2}}(\mathbf{k})\varphi_{B_{1}}(\mathbf{k}'),$$

we obtain from the gap Eq. (21) the following expressions for the intraband gap functions:

$$\widetilde{\Delta}_{\lambda\lambda} = \eta_{\lambda\lambda}^{A_1} \varphi_{A_1}(\boldsymbol{k}) + \eta_{\lambda\lambda}^{B_1} \varphi_{B_1}(\boldsymbol{k}) + \eta_{\lambda\lambda}^{B_2} \varphi_{B_2}(\boldsymbol{k}), \qquad (27)$$

and also for the interband gap functions:

$$\widetilde{\Delta}_{+-} = \eta_{+-}^{A_1} \varphi_{A_1}(\boldsymbol{k}) + \eta_{+-}^{B_1} \varphi_{B_1}(\boldsymbol{k}) + \eta_{+-}^{B_2} \varphi_{B_2}(\boldsymbol{k}) + \eta_{+-}^{E} \varphi_{E}(\boldsymbol{k}).$$
(28)

 $\widetilde{\Delta}_{-+}$  can be obtained from  $\widetilde{\Delta}_{+-}$  using Eq. (20). The expansion coefficients  $\eta^{\Gamma}_{\lambda\lambda'}(q)$  play the role of the order-parameter components.

In a general nonuniform case and at arbitrary values of the SO band splitting, and the coupling constants  $V_g$  and  $V_u$  [Eq. (22)], the gap Eq. (21) yields a set of coupled equations for the eleven components of the order parameter. In order to demonstrate the possibility of inhomogeneous solutions even in the absence of an external magnetic field, it is sufficient to

retain only the interband components in the  $A_1$  and E channels. To turn off the intraband pairing, we assume that  $V_g < 0$  (i.e., the isotropic channel is repulsive), and introduce the notations  $\eta_{+-}^{A_1} = \eta$  and  $\eta_{+-}^{E} = \xi$ . Then, using the symmetry properties (20), one can write

$$\Delta_{+-}(\boldsymbol{k},\boldsymbol{q}) = \eta(\boldsymbol{q})\varphi_{A_1}(\boldsymbol{k}) + \boldsymbol{\xi}(\boldsymbol{q})\varphi_E(\boldsymbol{k}),$$
$$\widetilde{\Delta}_{-+}(\boldsymbol{k},\boldsymbol{q}) = -\eta(\boldsymbol{q})\varphi_{A_1}(\boldsymbol{k}) + \boldsymbol{\xi}(\boldsymbol{q})\varphi_E(\boldsymbol{k}).$$
(29)

The linearized gap equations take the form

$$\eta = S^{\eta\eta}\eta + S_a^{\eta\xi}\xi_a, \quad \xi_a = S_a^{\eta\xi}\eta + S_{ab}^{\xi\xi}\xi_b, \tag{30}$$

where a, b=1, 2, and

$$S^{\eta\eta}(\boldsymbol{q}) = V_{u}T\sum_{n} \int \frac{d^{3}\boldsymbol{k}}{(2\pi)^{3}}\varphi_{A_{1}}^{2}(\boldsymbol{k})G_{+}G_{-},$$

$$S_{a}^{\eta\xi}(\boldsymbol{q}) = V_{u}T\sum_{n} \int \frac{d^{3}\boldsymbol{k}}{(2\pi)^{3}}\varphi_{A_{1}}(\boldsymbol{k})\varphi_{E,a}(\boldsymbol{k})G_{+}G_{-},$$

$$S_{ab}^{\xi\xi}(\boldsymbol{q}) = V_{u}T\sum_{n} \int \frac{d^{3}\boldsymbol{k}}{(2\pi)^{3}}\varphi_{E,a}(\boldsymbol{k})\varphi_{E,b}(\boldsymbol{k})G_{+}G_{-}.$$

Here the product of the Green's functions is  $G_+G_-=G_+(\mathbf{k}+\mathbf{q},\omega_n)G_-(-\mathbf{k},-\omega_n)$ . At  $\mathbf{q}=0$ , one obtains  $S_a^{\eta\xi}=0$ , which means that the  $A_1$  and E channels are decoupled. The critical temperature of the phase transition in a uniform superconducting state is the same for  $\eta$  and  $\boldsymbol{\xi}$ :

$$T_{c0} = T_{c0}^{\text{BCS}} - \frac{7\zeta(3)}{16\pi^2 T_{c0}}\alpha^2,$$
(31)

where  $T_{c0}^{BCS} = (2e^C/\pi)\omega_c \exp(-1/N_FV_u)$  is the standard BCS expression for the critical temperature in the absence of SO band splitting (i.e., at  $\alpha = 0$ ),  $\zeta(x)$  is the Riemann zetafunction,  $C \approx 0.577$  is Euler's constant, and  $N_F$  is the density of states at the Fermi level (we neglect the difference between the densities of states in the two bands). It is assumed that  $\alpha \leq T_{c0}$ ; otherwise the interband pairing is suppressed by the same mechanism that suppresses the singlet pairing in centrosymmetric superconductors. Indeed, the SO band splitting enters the Green's functions and the gap equations in exactly the same way as the Zeeman field does in the centrosymmetric case.

The actual critical temperature of the superconducting transition is higher than  $T_{c0}$ . Keeping the lowest terms in the gradient expansion in Eq. (30), we obtain

$$\left[a(T - T_{c0}) + Kq^{2}\right]\eta + Kq_{i}\xi_{i} = 0,$$
  
$$\widetilde{K}q_{i}\eta + \left[a(T - T_{c0})\delta_{ij} + \frac{K}{2}(\delta_{ij}q^{2} + 2q_{i}q_{j})\right]\xi_{j} = 0, \quad (32)$$

where  $a=N_F/T_{c0}$ ,  $K=7\zeta(3)N_Fv_F^2/32\pi^2T_{c0}^2$ , and  $\tilde{K} = 2\sqrt{2}K\alpha/v_F$ . The linear in q terms, which mix the two channels, correspond to the Lifshitz invariant in the Ginzburg-Landau free energy. In the coordinate representation, this invariant has the following form:

$$F_L = \widetilde{K} [\eta^* (\boldsymbol{D}\boldsymbol{\xi}) + (\boldsymbol{\xi}^* \boldsymbol{D}) \eta], \qquad (33)$$

where  $D = -i\nabla$ , or, in the presence of magnetic field,  $D = -i\nabla + (2e/c)A$ . It is easy to see that this expression satisfies all symmetry requirements. In particular, it is invariant under time-reversal operation, which in the band representation is expressed as  $\tilde{\Delta}_{\lambda_1\lambda_2}(\mathbf{k}) \rightarrow \tilde{\Delta}^*_{\lambda_2\lambda_1}(\mathbf{k})$ . According to Eq. (29), the order-parameter components transform under time reversal as follows:  $\eta \rightarrow -\eta^*$ ,  $\boldsymbol{\xi} \rightarrow \boldsymbol{\xi}^*$ .

Seeking the order parameter in the form

$$\eta(\mathbf{r}) = \eta_0 e^{iqx}, \quad \xi(\mathbf{r}) = \xi_0 e^{iqx}(1,0), \quad (34)$$

we obtain the following expression for the critical temperature as a function of q:

$$a(T - T_{c0}) = -\frac{5}{4}Kq^2 + \frac{1}{2}Kq\sqrt{32\left(\frac{\alpha}{v_F}\right)^2 + \frac{1}{4}q^2}.$$
 (35)

This function has a maximum at finite  $q=q_0$ , where

$$q_0 = c_1 \frac{\alpha}{v_F},\tag{36}$$

with  $c_1 \approx 1.15$ . The corresponding critical temperature is

$$T_c = T_{c0} + c_2 \frac{K}{a} \left(\frac{\alpha}{v_F}\right)^2,\tag{37}$$

where  $c_2 \approx 1.62$ . Thus, the nonuniform superconducting phase described by Eq. (34) has a higher critical temperature than the uniform state.

It is instructive to interpret our results using the spin representation of the order parameter:

$$\Delta_{\alpha\beta}(\boldsymbol{k},\boldsymbol{q}) = \sum_{\lambda_1\lambda_2} u_{\alpha\lambda_1}(\boldsymbol{k})\Delta_{\lambda_1\lambda_2}(\boldsymbol{k},\boldsymbol{q})u_{\beta\lambda_2}(-\boldsymbol{k})$$
$$= -\left[\hat{u}(\boldsymbol{k})\hat{\hat{\Delta}}(\boldsymbol{k},\boldsymbol{q})\hat{u}^{\dagger}(\boldsymbol{k})(i\hat{\sigma}_2)\right]_{\alpha\beta}.$$
(38)

The interband elements [see Eq. (29)] are translated into the spin representation as follows:

$$\Delta_{\alpha\beta}(\boldsymbol{k},\boldsymbol{q}) = (i\boldsymbol{\sigma}\boldsymbol{\sigma}_2)_{\alpha\beta}\boldsymbol{d}(\boldsymbol{k},\boldsymbol{q}), \qquad (39)$$

where

$$d_x = -i \eta(\boldsymbol{q}) \varphi_{A_1}(\boldsymbol{k}) \hat{k}_x, \quad d_y = -i \eta(\boldsymbol{q}) \varphi_{A_1}(\boldsymbol{k}) \hat{k}_y,$$
$$d_z = -\boldsymbol{\xi}(\boldsymbol{q}) \varphi_E(\boldsymbol{k}). \tag{40}$$

Therefore, the pairing symmetry in our model is purely spin triplet with  $d(k,q) \perp \gamma(k)$ .

The Cooper pairs in the nonuniform state are composed of electrons from different SO-split bands, and the order parameter is modulated with the wave vector  $q_0 \sim (\alpha/T_{c0})\xi_0^{-1}$  (here  $\xi_0$  is the coherence length). This effect formally resembles the nonuniform mixed-parity (NMP) state in centrosymmetric superconductors and superfluids in the presence of magnetic field, which was discussed in Refs. 14 and 15. The reason is that, as was mentioned above, the SO band splitting in the noncentrosymmetric case affects the interband pairing of electrons of opposite helicity in the same way as the Zee-

man field in centrosymmetric superconductors affects the usual BCS pairing between electrons of opposite spin. However, the NMP state originates from the triplet interaction channel introduced in the model along with the singlet channel. In contrast, the inhomogeneous superconducting state in the noncentrosymmetric case arises from a purely triplet pairing interaction [see the second line in Eq. (22)], which acquires both k-even and k-odd components in the band representation.

#### **IV. CONCLUSIONS**

We come to the conclusion that nonuniform superconducting states can exist in noncentrosymmetric superconductors even in the absence of external magnetic field. Experimentally, the zero-field nonuniform states discussed in this paper can only be observed in the noncentrosymmetric compounds with the SO band splitting smaller than the superconducting critical temperature. To the best of the authors' knowledge, in all noncentrosymmetric compounds discovered to date, the relation between the two energy scales is exactly the opposite: the SO band splitting exceeds all superconducting energy scales by orders of magnitude, completely suppressing the interband pairing both uniform and nonuniform.

We would like to note that the Lifshitz invariant considered in Sec. III is different from those discussed previously in the literature (Refs. 7 and 8). On the other hand, the Lifshitz invariants given by Eq. (15) for the crystal with cubic symmetry should exist also for a superconducting state with the order parameter transforming according to a multidimensional representation in crystals with other point symmetry groups. For instance, if the order parameters  $\eta_1$ ,  $\eta_2$  transform according to a two-dimensional representation of the point

group  $D_6$  (Ref. 7) (or the point group  $D_4$ ), then the Lifshitz invariant has the following form:

$$F_{L} = i\tilde{K}(\eta_{1}^{*}D_{z}\eta_{2} - \eta_{2}^{*}D_{z}\eta_{1}), \qquad (41)$$

where  $\tilde{K}$  is a real constant. Note that the corresponding invariant for the two-dimensional representation of  $C_{4v}$  is absent because it changes sign under reflections in the planes perpendicular to the *x* and *y* axes.

As pointed out in Ref. 7 an invariant of the form (41) should also exist if the order parameters  $\eta_1$ ,  $\eta_2$  are transformed according to two one-dimensional representations of different parity, in the case where the superconducting state arises from a centrosymmetric normal state as a result of parity violating pairing interaction. The corresponding microscopic theory can be easily developed.

Yet another possibility is related to the case of a superconducting state with two intraband components,  $\eta_+$  and  $\eta_-$ , of the same symmetry in a tetragonal crystal (Ref. 8). Then the Lifshitz invariant has the form:

$$F_{L} = i\tilde{K}(\eta_{+}^{*}D_{z}\eta_{-} - \eta_{-}^{*}D_{z}\eta_{+}).$$
(42)

Although this term satisfies all symmetry requirements and is therefore possible on phenomenological grounds, it is absent in our microscopic models. The derivation of such invariants would probably require more complicated theoretical constructions.

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- <sup>1</sup>E. Bauer, G. Hilscher, H. Michor, Ch. Paul, E. W. Scheidt, A. Gribanov, Yu. Seropegin, H. Noël, M. Sigrist, and P. Rogl, Phys. Rev. Lett. **92**, 027003 (2004).
- <sup>2</sup>V. M. Edelstein, J. Phys.: Condens. Matter 8, 339 (1996).
- <sup>3</sup>V. Barzykin and L. P. Gorkov, Phys. Rev. Lett. **89**, 227002 (2002).
- <sup>4</sup>D. F. Agterberg, Physica C **387**, 13 (2003).
- <sup>5</sup>A. I. Larkin and Yu. N. Ovchinnikov, Zh. Eksp. Teor. Fiz. **47**, 1136 (1964) [Sov. Phys. JETP **20**, 762 (1965)].
- <sup>6</sup>P. Fulde and R. A. Ferrell, Phys. Rev. 135, A550 (1964).
- <sup>7</sup>V. P. Mineev and K. V. Samokhin, Zh. Eksp. Teor. Fiz. **105**, 747 (1994) [JETP **78**, 401 (1994)].
- <sup>8</sup>K. V. Samokhin, E. S. Zijlstra, and S. K. Bose, Phys. Rev. B **69**, 094514 (2004); [ **70**, 069902(E) (2004) (erratum)].

- <sup>9</sup>V. P. Mineev and K. V. Samokhin, *Introduction to Unconventional Superconductivity* (Gordon and Breach, London, 1999).
- <sup>10</sup>K. V. Samokhin, Phys. Rev. B **70**, 104521 (2004).
- <sup>11</sup>P. A. Frigeri, D. F. Agterberg, A. Koga, and M. Sigrist, Phys. Rev. Lett. **92**, 097001 (2004); [ **93**, 099903(E) (2004) (erratum)].
- <sup>12</sup>K. V. Samokhin and V. P. Mineev, Phys. Rev. B 77, 104520 (2008).
- <sup>13</sup>L. D. Landau and E. M. Lifshitz, *Quantum Mechanics* (Butterworth-Heinemann, Oxford, 2002).
- <sup>14</sup>A. G. Lebed, Phys. Rev. Lett. **96**, 037002 (2006).
- <sup>15</sup>K. V. Samokhin and M. S. Mar'enko, Phys. Rev. Lett. 97, 197003 (2006).