

Massless collective excitations in frustrated multiband superconductors

Keita Kobayashi,¹ Masahiko Machida,^{1,2} Yukihiro Ota,³ and Franco Nori^{3,4}¹*CCSE, Japan Atomic Energy Agency, 5-1-5 Kashiwanoha, Kashiwa, Chiba 277-8587, Japan*²*Computational Materials Science Research Team, RIKEN AICS, Kobe, Hyogo 650-0047, Japan*³*CEMS, RIKEN, Saitama 351-0198, Japan*⁴*Physics Department, University of Michigan, Ann Arbor, Michigan 48109-1040, USA*

(Received 2 October 2013; revised manuscript received 16 December 2013; published 31 December 2013)

We study collective excitations in three- and four-band superconductors with interband frustration, which causes neither 0 nor π interband phases in the superconducting state. Using a low-energy spin Hamiltonian originating from a multiband tight-binding model, we find that mass reduction of a Leggett mode occurs in a wide parameter region of this four-band system. As a limiting case, we have a massless Leggett mode. This massless mode is related to the fact that the mean-field energy does not depend on a relative phase of superconducting order parameters. In other words, we find a link of the massless mode with a degeneracy between a time-reversal-symmetry-breaking state (neither 0 nor π phases) and a time-reversal-symmetric state (either 0 or π phases). Therefore, the mass of collective modes characterizes well the time-reversal symmetry in frustrated multiband superconductors.

DOI: [10.1103/PhysRevB.88.224516](https://doi.org/10.1103/PhysRevB.88.224516)

PACS number(s): 74.20.-z, 03.75.Kk, 67.10.-j, 74.70.Xa

I. INTRODUCTION

Frustration leads to intriguing phenomena in different physical systems [1,2]. Multiband superconductors/superfluids, such as iron-based materials [3,4] and multicomponent ultracold atomic gases [5–7], can be frustrated many-body systems. Frustration in these systems originates from competitive interaction between different bands/components, not different spatial sites. This curious *interband frustration* allows a time-reversal-symmetry breaking (TRSB) superconducting state [8–10].

Collective excitations characterize well an ordered state in many-body quantum systems. The Leggett mode [11–17] is a characteristic collective excitation in multiband superconductivity, as well as the Nambu-Goldstone (NG) mode associated with U(1)-symmetry breaking, and has been studied in multiband systems such as magnesium diboride [18], iron-based materials [19], and atomic gases on a honeycomb optical lattice [20,21]. The mass of the Leggett mode strongly depends on interband couplings [12]. A recent striking result [14] is that the mass in a three-band system vanishes at the boundary between a time-reversal symmetric (TRS) state and a TRSB state, changing the strength of the interband coupling.

In this paper, we study the connection between interband frustration and the mass of collective excitations. To study properties depending on the number of bands, we focus on two cases, as seen in Fig. 1. First, we examine a three-band system as a minimal model for showing the interband frustration. Second, we study a four-band system as an example which shows a feature different from the three-band system. Our approach is to make a map from a multiband tight-binding model to an effective frustrated spin Hamiltonian. An analogy with a classical spin system is useful for examining multiband superconductors [10].

A mean-field theory of the effective spin Hamiltonian allows us to calculate the superconducting-phase configurations and the collective excitations. Varying the strength of the interband couplings, we obtain a phase diagram of the superconducting state. The massless Leggett mode is found at the phase boundaries between the TRSB and TRS states.

This result is consistent with the result by Lin and Hu [14]. The main result in this paper is that in the four-band system a massless Leggett mode occurs in a parameter region other than the TRSB-TRS phase boundaries. In this region, the mean-field energy for a TRSB state is equal to the one for a TRS state. Therefore, this massless behavior is related to the degenerate superconducting states. Moreover, we characterize this massless mode, from the viewpoint of interband symmetry. Thus, we claim that the mass of collective excitations gives an insight into spontaneous-symmetry breaking in the presence of interband frustration.

This paper is organized as follows. The effective spin Hamiltonian is derived from a multiband tight-binding model in Sec. II. The formulas for calculating the superconducting order parameter and the collective excitations are derived, with mean-field approximation. In Sec. III, we solve the resultant formulas in a spatially homogeneous case. We show that the massless behaviors of the Leggett mode are associated with energy degeneracy between the TRSB state and the TRS state. Furthermore, we discuss an effect of quantum fluctuations on the massless modes in Sec. IV. Section V is devoted to the summary.

II. EFFECTIVE HAMILTONIAN WITH ANTIFERROMAGNETIC XY INTERACTION

An effective Hamiltonian is derived from a multiband tight-binding model, via the second order perturbation. This effective model explicitly shows the presence of interband frustration, in terms of antiferromagnetic *XY* interaction. Using the mean-field approximation, we show the formulas for calculating the superconducting order parameters and the collective excitations in a spatially homogeneous case. We also define a witness for the TRSB state, scalar chiral order parameter. In the subsequent section, we will calculate these equations numerically.

The Hamiltonian is

$$H = \sum_{\alpha} \sum_{\sigma=\uparrow,\downarrow} h_{\alpha,\sigma} + \sum_{\alpha,\alpha'} v_{\alpha,\alpha'}, \quad (1)$$

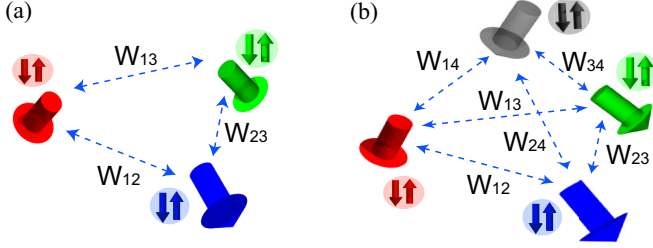


FIG. 1. (Color online) Schematic diagrams of interband configurations in (a) three- and (b) four-band systems. Each large arrow indicates the orientation of a pseudospin formed by a fermion-pair particle on a band. Since interband couplings $W_{\alpha\alpha'}$ are repulsive, an antiferromagnetic interaction occurs between the pseudospins. See Eq. (4).

with

$$h_{\alpha,\sigma} = - \sum_{\langle i,j \rangle} t_{\alpha} c_{\alpha,\sigma,i}^{\dagger} c_{\alpha,\sigma,j} - \sum_i \mu c_{\alpha,\sigma,i}^{\dagger} c_{\alpha,\sigma,i}, \quad (2)$$

$$v_{\alpha,\alpha'} = \sum_i W_{\alpha\alpha'} c_{\alpha,\uparrow,i}^{\dagger} c_{\alpha,\downarrow,i}^{\dagger} c_{\alpha',\downarrow,i} c_{\alpha',\uparrow,i}. \quad (3)$$

The spatial site is $\mathbf{i} = (i_x, i_y, i_z)$. The electron creation (annihilation) operator is $c_{\alpha,\sigma,i}^{\dagger}$ ($c_{\alpha,\sigma,i}$) for the α th band on \mathbf{i} . The hopping matrix element and the chemical potential are, respectively, t_{α} and μ . The intraband coupling $W_{\alpha\alpha}$ is negative (attractive interaction), while the interband coupling $W_{\alpha\alpha'}$ ($\alpha \neq \alpha'$) is positive (repulsive interaction).

Our approach for deriving an effective model from Eq. (1) is the second-order Brillouin-Wigner perturbation. Since strong intraband coupling produces condensates, our choice of a free Hamiltonian is $H_0 = \sum_{\alpha} v_{\alpha,\alpha}$. The attractive-repulsive transformation [22] makes Eq. (1) a half-filled system. This transformation is defined by $c_{\alpha,\uparrow,i} = \bar{c}_{\alpha,\uparrow,i}$ and $c_{\alpha,\downarrow,i} = \exp(-i\mathbf{q} \cdot \mathbf{x}_i) \bar{c}_{\alpha,\downarrow,i}^{\dagger}$, with a reciprocal vector \mathbf{q} satisfying $\exp[i\mathbf{q} \cdot (\mathbf{x}_{i+\mathbf{l}} - \mathbf{x}_i)] = -1$, for $l = x, y, z$, where $\mathbf{x}_i = \sum_l i_l \mathbf{a}_l$ and $\mathbf{l} = \mathbf{a}_l / |\mathbf{a}_l|$. The lattice vector along the l axis is \mathbf{a}_l . The ground-state subspace of H_0 is $\mathcal{H}_g = \otimes_{\alpha,i} \{ \bar{c}_{\alpha,\uparrow,i}^{\dagger} |\bar{0}\rangle, \bar{c}_{\alpha,\downarrow,i}^{\dagger} |\bar{0}\rangle \}$, and the excited-state subspace is $\mathcal{H}_e = \otimes_{\alpha,i} \{ |\bar{0}\rangle, \bar{c}_{\alpha,\downarrow,i}^{\dagger} \bar{c}_{\alpha,\uparrow,i}^{\dagger} |\bar{0}\rangle \}$. The ket vector $|\bar{0}\rangle$ is defined by $\bar{c}_{\alpha,\sigma,i} |\bar{0}\rangle = 0$. The effective Hamiltonian is $H_{\text{eff}} = PVP - (PVP)H_0^{-1}(QVP)$, with $V = H - H_0$. The projector onto \mathcal{H}_g (\mathcal{H}_e) is P (Q).

Let us write H_{eff} in terms of the pseudospin 1/2 operators defined by $\bar{S}_{\alpha,i}^{(+)} = \bar{c}_{\alpha,\uparrow,i}^{\dagger} \bar{c}_{\alpha,\downarrow,i}$, $\bar{S}_{\alpha,i}^{(-)} = [\bar{S}_{\alpha,i}^{(+)}]^{\dagger}$, and $\bar{S}_{\alpha,i}^{(z)} = (\bar{c}_{\alpha,\uparrow,i}^{\dagger} \bar{c}_{\alpha,\uparrow,i} - \bar{c}_{\alpha,\downarrow,i}^{\dagger} \bar{c}_{\alpha,\downarrow,i})/2$. These operators represent a fermion-pair particle. The second perturbation term leads to the Heisenberg Hamiltonian with exchange interaction $J_{\alpha} = 2t_{\alpha}^2/|W_{\alpha\alpha}|$. The contribution from $W_{\alpha\alpha'}$ ($\alpha \neq \alpha'$) appears as the first perturbation term since $Pv_{\alpha,\alpha'}Q = 0$ for $\alpha \neq \alpha'$. Thus,

$$H_{\text{eff}} = \sum_{\alpha} \sum_{\langle i,j \rangle} J_{\alpha} [\bar{S}_{\alpha,i}^{(z)} \bar{S}_{\alpha,j}^{(z)} + \bar{S}_{\alpha,i}^{(+)} \bar{S}_{\alpha,j}^{(-)}] + \sum_{\alpha \neq \alpha'} \sum_i W_{\alpha\alpha'} \bar{S}_{\alpha,i}^{(+)} \bar{S}_{\alpha',i}^{(-)} - \sum_{\alpha,i} 2\bar{\mu}_{\alpha} \bar{S}_{\alpha,i}^{(z)}, \quad (4)$$

with $\bar{\mu}_{\alpha} = \mu + |W_{\alpha\alpha}|/2$. The interband interaction is regarded as an antiferromagnetic XY interaction.

We examine Eq. (4), using the mean-field approach with spatial uniformity. Let us rewrite the pseudospin-1/2 operators, in terms of $b_{\alpha,i}$, such that $\bar{S}_{\alpha,i}^{(+)} = \exp(-i\mathbf{q} \cdot \mathbf{x}_i) b_{\alpha,i}$ and $\bar{S}_{\alpha,i}^{(z)} = (1/2) - b_{\alpha,i}^{\dagger} b_{\alpha,i}$. We find that $[b_{\alpha,i}, b_{\alpha',i'}^{\dagger}] = (1 - b_{\alpha,i}^{\dagger} b_{\alpha,i}) \delta_{i,i'} \delta_{\alpha,\alpha'}$ and $b_{\alpha,i}^2 = 0$. In the dilute limit $\langle b_{\alpha,i}^{\dagger} b_{\alpha,i} \rangle \ll 1$, $b_{\alpha,i}$ can be regarded as a standard bosonic operator. Using $\langle b_{\alpha,i} \rangle = \Delta_{\alpha,i}$, we obtain the mean-field energy E_c as a function of $\Delta_{\alpha,i}$. For the uniform order parameters ($\Delta_{\alpha,i} = \Delta_{\alpha}$), Δ_{α} is determined by $(\partial E_c / \partial \Delta_{\alpha}^*) = 0$, namely,

$$-2J_{\alpha} D (1 - 2|\Delta_{\alpha}|^2) \Delta_{\alpha} + \sum_{\alpha' \neq \alpha} W_{\alpha\alpha'} \Delta_{\alpha'} - v_{\alpha} \Delta_{\alpha} = 0, \quad (5)$$

where $v_{\alpha} = 2DJ_{\alpha} - 2\bar{\mu}_{\alpha}$ and D is the dimension of the system. The collective excitations for momentum \mathbf{k} are calculated, combining the resultant gaps with the Bogolubov de-Genes equation

$$T_{\mathbf{k}} \mathbf{Y}_{\mathbf{k}} = \omega_{\mathbf{k}} \mathbf{Y}_{\mathbf{k}}, \quad (6)$$

with $T_{\mathbf{k}} = \tau_z \otimes \mathcal{L} + \tau_x \otimes i\text{Im} \mathcal{M} + \tau_y \otimes i\text{Re} \mathcal{M}$. $\mathbf{Y}_{\mathbf{k}}$ is a $2N$ -complex vector, where N is the number of bands. The 2×2 Pauli matrices (τ_x, τ_y, τ_z) represent the so-called particle-hole symmetry of the Bogoliubov-de Gennes equation. The $N \times N$ matrices \mathcal{L} and \mathcal{M} are defined as

$$\mathcal{L}_{\alpha\alpha'} = -2\delta_{\alpha,\alpha'} \sum_l [\varepsilon_{\alpha,k_l} - 2(\varepsilon_{\alpha,k_l} - \varepsilon_{\alpha,0}) |\Delta_{\alpha}|^2] - \delta_{\alpha,\alpha'} v_{\alpha} + (1 - \delta_{\alpha,\alpha'}) W_{\alpha\alpha'}, \quad (7)$$

$$\mathcal{M}_{\alpha\alpha'} = \delta_{\alpha,\alpha'} \sum_l 4\varepsilon_{\alpha,k_l} \Delta_{\alpha}^2. \quad (8)$$

The coefficient ε_{α,k_l} is the Fourier-transformed hopping matrix element $\varepsilon_{\alpha,k_l} = J_{\alpha} \cos(k_l a_l)$, with lattice constant $a_l (= |\mathbf{a}_l|)$.

The superconducting states are classified by the scalar chiral order parameter [23,24]

$$\chi = \sum_{\alpha_1 < \alpha_2 < \alpha_3} |(\bar{S}_{\alpha_1} \cdot (\bar{S}_{\alpha_2} \times \bar{S}_{\alpha_3}))|. \quad (9)$$

Under the mean-field approximation and the dilute limit, the components of the pseudospin 1/2 vector \bar{S}_{α} are $\bar{S}_{\alpha} \simeq \langle \bar{S}_{\alpha} \rangle = {}^t(\Delta_{\alpha}^R, \Delta_{\alpha}^I, 1/2 - |\Delta_{\alpha}|^2) \simeq {}^t(\Delta_{\alpha}^R, \Delta_{\alpha}^I, 1/2)$, where Δ_{α}^R and Δ_{α}^I are, respectively, the real and the imaginary parts of Δ_{α} . The interband phases (e.g., $\Delta_1^R \Delta_2^I - \Delta_1^I \Delta_2^R$) are important for determining the TRSB state. We sum up such quantities over all the band indices in Eq. (9). We note that $\chi = 0$ when $\Delta_{\alpha}^I = 0$ for all α .

III. MASS REDUCTION OF A LEGGETT MODE BY INTERBAND FRUSTRATION

We calculate the scalar chiral order parameter on a 2D square lattice ($D = 2$ and $a_l = a$), numerically solving Eq. (5), according to the imaginary-time evolution method [25,26]. We also evaluate the collective modes by direct diagonalization of Eq. (6). Here, we consider in a highly symmetric case $t_{\alpha} = t$ for simplicity and focus on a strong intraband interaction case, $W_{\alpha\alpha}/t = -6$, to ensure the validity of Eq. (4). Throughout

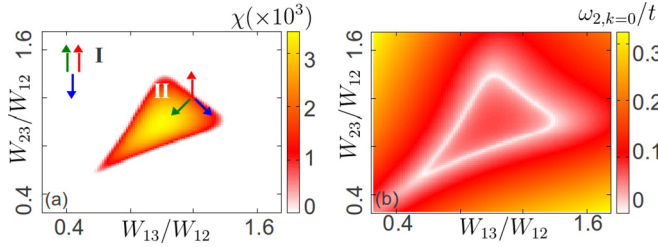


FIG. 2. (Color online) Density profiles of (a) a scalar chiral order parameter and (b) Leggett-mode mass, in a three-band superconductor, varying interband couplings W_{13}/W_{12} and W_{23}/W_{12} . In (a), the arrows show typical superconducting-phase configurations.

this paper, we set $J_\alpha/t = J/t = 1/3$. The condensate particle density is also fixed as $n_c = \sum_\alpha |\Delta_\alpha|^2 = 0.1$. The number of the collective modes depends on N . We will denote the NG mode as $\omega_{1,k}$. The others correspond to the Leggett modes.

First, we show the results for the three-band case. Figure 2(a) shows the presence of different parameter regions. In region I the TRS states occur ($\chi = 0$), whereas in region II the TRSB states occur ($\chi \neq 0$). In region I a sign change (antiparallel arrangement of pseudospins) occurs between the gaps. In region II a typical phase configuration is that each relative superconducting phase is $2\pi/3$. In other words, each pseudospin directs from the center to the vertex of an equilateral triangle. Figure 2(b) shows that the mass of the Leggett mode ($\omega_{2,k=0}$) vanishes at the TRSB-TRS phase boundaries. These results are consistent with the results of a weak-coupling model [14]. The phase transition between the TRS and the TRSB state is the second-order one, as shown by Lin and Hu [14]. The fluctuation developed at the critical point may lead to this massless behavior.

Now, let us show the four-band case. We change W_{13} and W_{24} , with fixed W_{12}, W_{23}, W_{34} , and W_{14} . From the viewpoint of Fig. 1, the length of four sides in a tetrahedron is fixed. First, we show similar features to the three-band case. Figure 3(a1) shows the results for $W_{12} = W_{34} = 0.23$ and $W_{23} = W_{14} = 0.2$. The TRSB state appears in region II, whereas the TRS states occur in the other regions. The phase configuration in region II is similar to the three-band case, although two of the pseudospins are aligned (0-phase shift). We also find that the mass of the Leggett mode vanishes at the TRSB-TRS phase boundaries, as seen in Fig. 3(b1). Changing the condition for the fixed interband couplings, different features appear. Let us consider the case of $W_{12} = W_{23} = 0.23$ and $W_{34} = W_{14} = 0.2$. Figure 3(a2) shows the presence of a curious area (region III), where the time-reversal symmetry is fully broken. In other words, every relative phase is neither 0 nor π . Figure 3(b2) shows that the mass of the Leggett mode is close to zero inside this region. We can also find that $\omega_{2,k=0}$ and $\omega_{3,k=0}$ become zero near the phase boundaries between II and III (no figure shown for $\omega_{3,k}$). A more exotic feature appears in the identical interband interaction $W_{12} = W_{23} = W_{34} = W_{14} = 0.2$. Figure 3(a3) shows that χ randomly changes in region III [26]. $\omega_{2,k}$ is massless in this wide area, not restricted near the phase boundaries.

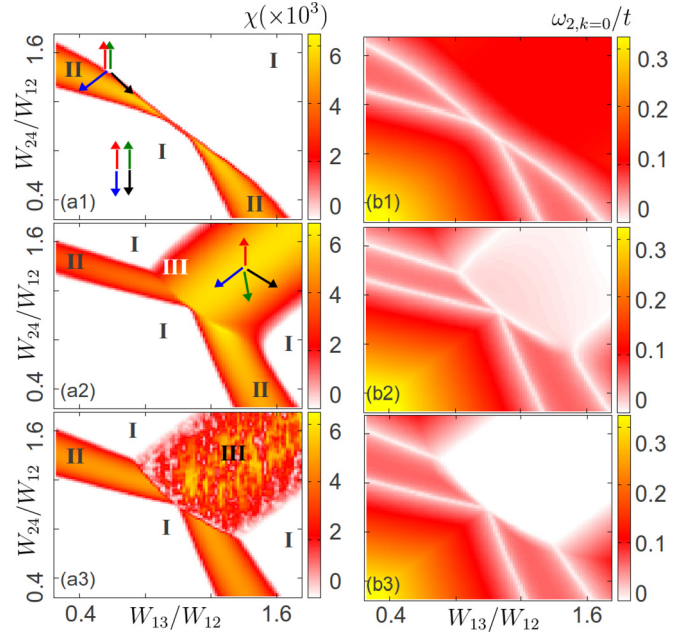


FIG. 3. (Color online) Density profiles of (a1,a2,a3) a scalar chiral order parameter and (b1,b2,b3) Leggett-mode mass, in a four-band superconductor, varying interband couplings W_{13} and W_{24} . The other interband couplings are fixed as $W_{12} = W_{34} = 0.23$, $W_{23} = W_{14} = 0.2$ in (a1,b1), $W_{12} = W_{23} = 0.23$, $W_{34} = W_{14} = 0.2$ in (a2,b2), and $W_{12} = W_{23} = W_{34} = W_{14} = 0.2$ in (a3,b3). The arrows in (a1,a2) show typical superconducting-phase configurations like Fig. 2.

We examine region III in Fig. 3(a3) in detail. Since $W_{13} > W_{12}$, a π shift may occur between Δ_1 and Δ_3 . Similarly, the condition $W_{24} > W_{12}$ means $\Delta_4 = e^{\pm i\pi} \Delta_2$. Moreover, since $W_{12} = W_{34}$, the relative phase between Δ_1 and Δ_2 should be equal to the one between Δ_3 and Δ_4 . Therefore, we construct a solution of Eq. (5) in region III, with ansatz

$$\Delta = (|\Delta_+|, e^{i\phi} |\Delta_-|, e^{i\pi} |\Delta_+|, e^{i(\phi+\pi)} |\Delta_-|). \quad (10)$$

The global phase is fixed so that Δ_1 is real. Substituting this expression into Eq. (5), we find that $|\Delta_\pm| = (1/2)\sqrt{n_c} \pm (W_{13} - W_{24})/2JD$, but the relative phase is not fixed. This result indicates that the mean-field energy for Eq. (10) is independent of the continuous parameter ϕ , and a degeneracy exists between the TRSB and the TRS states. Thus, the massless behavior in region III is related to a degeneracy. The occurrence of such an exotic massless mode and a degeneracy between ground states were pointed out by several authors [27–30].

A symmetry analysis of Eq. (6) leads to insights into the massless Leggett mode. The identical interband couplings ($W_{12} = W_{23} = W_{34} = W_{14}$) and the order parameters [Eq. (10)] indicate the presence of a symmetric property in Eq. (6). We find that $\mathcal{L} = \mathbb{1} \otimes \mathcal{L}_0 + \eta_x \otimes \mathcal{L}_x$ and $\mathcal{M} = \mathbb{1} \otimes \mathcal{M}_0$, with the x component of the 2×2 Pauli matrices, η_x and complex 2×2 matrices \mathcal{L}_0 , \mathcal{L}_x , and \mathcal{M}_0 . Hence, η_x commutes with T_k . We mention that η_x corresponds to swap between the upper 2-band and the lower 2-band blocks. After

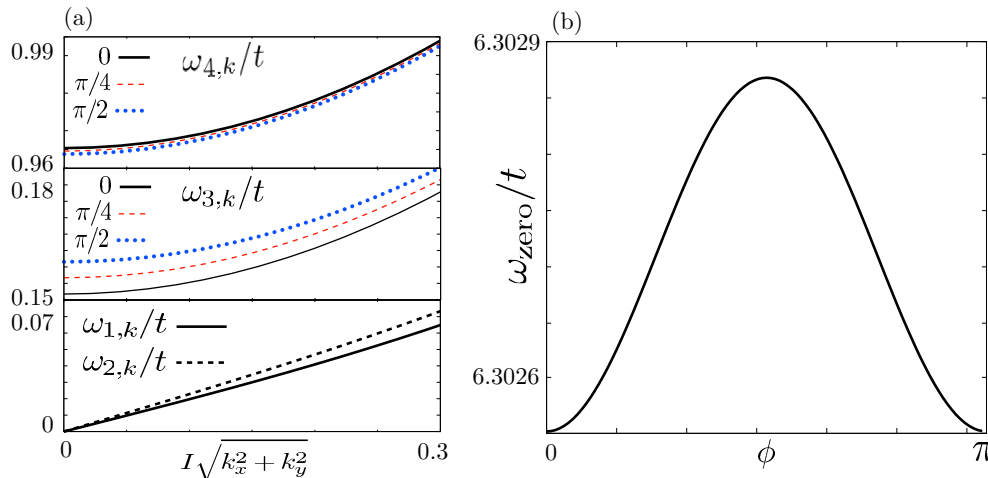


FIG. 4. (Color online) (a) Dispersion relations for collective excitations, with relative phases $\phi = 0, \pi/4, \pi/2$. $\omega_{1,k}$ and $\omega_{2,k}$ are independent of ϕ . (b) Zero-point energy of the collective excitations, varying ϕ . In both figures, interband couplings are set as $W_{13}/W_{12} = 1.2$, $W_{24}/W_{12} = 1.3$, and $W_{12} = W_{23} = W_{34} = W_{14} = 0.2$.

a permutation, we rewrite $T_{\mathbf{k}}$ as

$$T_{\mathbf{k}} = \frac{1 + \eta_x}{2} \otimes T_{+,k} + \frac{1 - \eta_x}{2} \otimes T_{-,k}, \quad (11)$$

with $T_{\pm,k} = \text{tr}_{\eta}[T_{\mathbf{k}}(1 \pm \eta_x)]/2$. The symbol tr_{η} means the trace over η basis. The characteristic polynomial of $T_{-,k}$ is written by $f(z) = \sum_{n=0}^4 c_n(\mathbf{k})z^{4-n}$, with $c_0 = 1$. Since we can find that the coefficients for $n = 1, 2, 3$ are zero when $\mathbf{k} = 0$, $T_{\mathbf{k}}$ has two zero modes, one of which is the NG mode, while the other of which is the massless Leggett mode. Thus, the present massless Leggett mode belongs to the same subspace as the NG mode, and is regarded as a quasi-NG mode.

IV. DISCUSSION

We refer to an effect of quantum fluctuations on the ground-state degeneracy. The simplest approach to take such corrections is to add the zero-point energy of the collective excitations to the mean-field energy. The correction can be written as $\omega_{\text{zero}} = \sum_{\alpha} \sum_{\mathbf{k}} \omega_{\alpha,k}/I$, with the total number I of the spatial sites. Let us examine this correction in region III of Fig. 3(a3). Figure 4(a) shows that $\omega_{3,k}$ and $\omega_{4,k}$ depend on ϕ , whereas the others not so. Figure 4(b) shows ω_{zero} has minimum values at either 0 or π . In other words, the massive collective modes in region III make a selection of a true ground state. The TRS state is preferable in region III, owing to ω_{zero} .

The above consideration indicates that our quasi-NG mode may obtain some mass originating from quantum fluctuations. This point is also discussed in a different system, spinor Bose-Einstein condensate [28]. Nevertheless, the mass of the Leggett mode is a good indicator of interband frustration. Indeed, our calculations show that the mass of the Leggett mode drastically reduces (almost to zero) when there is strong competition between the interband couplings, even though the ground-state degeneracy is absent. See region III of Fig. 3(b2), for example. In this region, only the TRSB state occurs; it means that strong interband frustration appears. Thus, although the Leggett mode does not become a complete massless mode

in the presence of quantum fluctuations, one may observe a significant mass reducing behavior of a Leggett mode. When the long-range Coulomb interaction exists, the situation becomes much clearer. Typically, the NG mode obtains the mass via the Anderson-Higgs mechanism; the massive plasma excitations may appear. However, since the Leggett modes are related to neutral superfluid-phase fluctuations [12], one may observe low-energy excitations related to the Leggett mode with tiny mass, whenever strong interband frustration exists. Therefore, we expect that the mass reducing behavior of the Leggett mode predicted by the present mean-field analysis is robust against quantum fluctuations and the gauge field. A more systematic study about different fluctuations will be an interesting future work.

V. SUMMARY

We have examined the collective excitations in three- and four-band superconductors. Using an effective spin Hamiltonian, we showed that interband frustration induces two kinds of massless Leggett modes, and clarified their physical origin. The mass of a collective mode characterizes well the time-reversal symmetry of frustrated multiband superconductors.

ACKNOWLEDGMENTS

We thank M. Okumura and H. Nakamura for useful discussions. This work was partially supported by MEXT Strategic Programs for Innovative Research, and the Computational Materials Science Initiative, Japan. We are indebted to T. Toyama for his support. Y.O. is partially supported by the Special Postdoctoral Researchers Program, RIKEN. F.N. acknowledges partial support from the ARO, RIKEN iTHES project, JSPS-RFBR Contract No. 12-02-92100, Grant-in-Aid for Scientific Research (S), MEXT Kakenhi on Quantum Cybernetics, and Funding Program for Innovative R&D on S&T.

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