Gap structure in noncentrosymmetric superconductors

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Gap structure in noncentrosymmetric superconductors with spin-orbit band splitting is studied using a microscopic model of pairing mediated by phonons and/or spin fluctuations. The general form of pairing interaction in the band representation is derived, which includes both the intraband and interband pairing terms. In the case of isotropic interaction (in particular, for a BCS-contact interaction), the interband pairing terms vanish identically at any magnitude of the band splitting. The effects of pairing interaction anisotropy are analyzed in detail for a metal of cubic symmetry with strong spin-orbit coupling. It is shown that if phonons are dominant then the gaps in two bands are isotropic, nodeless, and have in general different amplitudes. Applications to the $Li_2(Pd_{1-x},Pt_x)_3B$ family of noncentrosymmetric superconductors are discussed.

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I. INTRODUCTION

Superconducting materials without inversion symmetry have recently become a subject of considerable interest, both experimental and theoretical. Starting from $CePt_3Si$ (Ref. 1), the list of noncentrosymmetric superconductors has grown to include UIr (Ref. 2), $CeRhSi_3$ (Ref. 3), $CeIrSi_3$ (Ref. 4), Y_2C_3 (Ref. 5), $Li_2(Pd_{1-x},Pt_x)_3B$ (Ref. 6), KOs_2O_6 (Ref. 7), and other compounds. In most cases, the fundamental questions about the gap symmetry and the pairing mechanism remain unresolved.

The spin-orbit (SO) coupling of electrons with a noncentrosymmetric crystal lattice lifts spin degeneracy of the electron energy bands almost everywhere, which has important consequences for superconductivity: In the limit of strong SO coupling, the Cooper pairing between the electrons with opposite momenta occurs only if they are from the same nondegenerate band. This scenario is realized in $CePt_3Si$, where the SO band splitting exceeds the critical temperature by orders of magnitude.[8] The same is likely to be the case in other materials, for instance in $Li_2(Pd_{1-x},Pt_x)_3B$; see Ref. 9.

The pairing interaction between electrons is most naturally introduced using the exact band states,[8,10–12] which take into account all the effects of the crystal lattice potential and the SO coupling, see Sec. II. In the strong SO coupling limit, the order parameter is represented by a set of complex functions, one for each band, which makes the theory of noncentrosymmetric superconductors similar to that of usual multiband superconductors, see Ref. 13. An alternative approach based on the representation of the pairing interaction in terms of the pure spinor states unaffected by the SO coupling was developed in Refs. 14 and 15.

In a phenomenological multiband pairing Hamiltonian, the relative strength of pairing in different bands can be arbitrary. In this article, we go beyond the phenomenological description and study the gap structure in noncentrosymmetric superconductors under some fairly general assumptions about the microscopic mechanism of pairing. Specifically, we consider the interaction mediated by bosonic excitations (phonons and/or spin fluctuations). Starting with a microscopic expression for a momentum and frequency dependent pairing interaction, we derive the general form of the pairing interaction in the band representation, which contains both the intraband and interband pairing terms. The latter is shown to vanish identically in the case of isotropic BCS-contact interaction for any magnitude of the SO band splitting; see Sec. III. In general, the interband pairing is absent only in the limit of large band splitting; see Sec. IV.

In Sec. V, we present a detailed analysis of the possible gap structures in noncentrosymmetric superconductors of cubic symmetry, in a model which includes both the phonon and spin-fluctuation mediated interactions. The Conclusion contains a discussion of our results in the context of $Li_2(Pt_{1-x},Pt_x)_3B$ experiments.

II. BASIC DEFINITIONS

The Hamiltonian of noninteracting electrons in a noncentrosymmetric crystal has the following form:

$$H_0=\sum_{\boldsymbol{k}}[\epsilon_0(\boldsymbol{k})\delta_{\alpha\beta}+\boldsymbol{\gamma}(\boldsymbol{k})\boldsymbol{\sigma}_{\alpha\beta}]a^\dagger_{\boldsymbol{k}\alpha}a_{\boldsymbol{k}\beta}=\sum_{\boldsymbol{k}}\sum_{\lambda=\pm}\xi_\lambda(\boldsymbol{k})c^\dagger_{\boldsymbol{k}\lambda}c_{\boldsymbol{k}\lambda}, \tag{1}$$

where $\alpha,\beta=\uparrow,\downarrow$ are spin indices, $\boldsymbol{\sigma}$ are the Pauli matrices, $\xi_\lambda(\boldsymbol{k})=\epsilon_0(\boldsymbol{k})+\lambda|\boldsymbol{\gamma}(\boldsymbol{k})|$ are the band dispersion functions, and the sum over $\boldsymbol{k}$ is restricted to the first Brillouin zone. In Eq. (1) and everywhere below, summation over repeated spin indices is implied, while summation over the band indices is always shown explicitly. The SO coupling of electrons with the crystal lattice is described by the pseudovector $\boldsymbol{\gamma}(\boldsymbol{k})$, which satisfies $\boldsymbol{\gamma}(-\boldsymbol{k})=-\boldsymbol{\gamma}(\boldsymbol{k})$ and $(g\boldsymbol{\gamma})(g^{-1}\boldsymbol{k})=\boldsymbol{\gamma}(\boldsymbol{k})$, where g is any operation from the point group $\mathbb{G}$ of the crystal; see the examples below.

The Hamiltonian in the first line of Eq. (1) is diagonalized by the following transformation:

$$a_{\boldsymbol{k}\alpha}=\sum_{\lambda=\pm}u_{\alpha\lambda}(\boldsymbol{k})c_{\boldsymbol{k}\lambda}, \tag{2}$$

with the coefficients

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

$$u_{\downarrow\lambda}(\boldsymbol{k}) = \lambda\frac{\gamma_x + i\gamma_y}{\sqrt{2|\boldsymbol{\gamma}|(|\boldsymbol{\gamma}| + \lambda\gamma_z)}} \tag{3}$$

forming a unitary matrix $\hat{u}(\boldsymbol{k})$. The Fermi surfaces defined by the equations $\xi_\pm(\boldsymbol{k})=0$ are split, except for the points or lines where $\boldsymbol{\gamma}(\boldsymbol{k})=0$. The band dispersion functions $\xi_\lambda(\boldsymbol{k})$ are invariant with respect to all operations from $\mathbb{G}$, and also even in $\boldsymbol{k}$ due to time reversal symmetry: The states $|\boldsymbol{k},\lambda\rangle$ and $K|\boldsymbol{k},\lambda\rangle$ belong to $\boldsymbol{k}$ and $-\boldsymbol{k}$, respectively, and have the same energy. Here $K=i\hat{\sigma}_2K_0$ is the time reversal operation, and K_0 is the complex conjugation. One can write $K|\boldsymbol{k},\lambda\rangle = t_\lambda(\boldsymbol{k})|-\boldsymbol{k},\lambda\rangle$, where $t_\lambda(\boldsymbol{k})=-t_\lambda(-\boldsymbol{k})$ is a nontrivial phase factor.[10,11] For the eigenstates defined by expressions (3) we obtain

$$t_\lambda(\boldsymbol{k}) = \lambda\frac{\gamma_x(\boldsymbol{k}) - i\gamma_y(\boldsymbol{k})}{\sqrt{\gamma_x^2(\boldsymbol{k}) + \gamma_y^2(\boldsymbol{k})}}. \tag{4}$$

The momentum dependence of the SO coupling is determined by the crystal symmetry. For the cubic group $\mathbb{G}=\mathbf{O}$, which describes the point symmetry of $Li_2(Pd_{1-x},Pt_x)_3B$, the simplest form compatible with the symmetry requirements is

$$\boldsymbol{\gamma}(\boldsymbol{k}) = \gamma_0\boldsymbol{k}, \tag{5}$$

where γ_0 is a constant. For the point groups containing improper elements, i.e., reflections and rotation-reflections, expressions become more complicated. In the case of the full tetrahedral group $\mathbb{G}=\mathbf{T}_d$, which is relevant for Y_2C_3 and possibly KOs_2O_6, one has

$$\boldsymbol{\gamma}(\boldsymbol{k}) = \gamma_0[k_x(k_y^2 - k_z^2)\hat{x} + k_y(k_z^2 - k_x^2)\hat{y} + k_z(k_x^2 - k_y^2)\hat{z}]. \tag{6}$$

This is also known as the Dresselhaus interaction,[16] and was originally proposed to describe the SO coupling in bulk semiconductors of zinc-blende structure. For the tetragonal group $\mathbb{G}=\mathbf{C}_{4v}$, which is relevant for $CePt_3Si$, $CeRhSi_3$ and $CeIrSi_3$, the SO coupling is given by

$$\boldsymbol{\gamma}(\boldsymbol{k}) = \gamma_\perp(k_y\hat{x} - k_x\hat{y}) + \gamma_\parallel k_xk_yk_z(k_x^2 - k_y^2)\hat{z}. \tag{7}$$

In the purely two-dimensional case, setting $\gamma_\parallel=0$ one recovers the Rashba interaction,[17] which is often used to describe the effects of the absence of mirror symmetry in semiconductor quantum wells.

Now let us take into account an attractive interaction between electrons in the Cooper channel, using the basis of the exact eigenstates of the noninteracting problem. The most general form of the interaction Hamiltonian the band representation is

$$H_{\text{int}} = \frac{1}{2\mathcal{V}}\sum_{\boldsymbol{k}\boldsymbol{k}'\boldsymbol{q}}\sum_{\lambda_{1,2,3,4}} V_{\lambda_1\lambda_2\lambda_3\lambda_4}(\boldsymbol{k},\boldsymbol{k}';\boldsymbol{q}) \times c^\dagger_{\boldsymbol{k}+\boldsymbol{q},\lambda_1}c^\dagger_{-\boldsymbol{k},\lambda_2}c_{-\boldsymbol{k}',\lambda_3}c_{\boldsymbol{k}'+\boldsymbol{q},\lambda_4}. \tag{8}$$

We assume that the $\boldsymbol{q}$ dependence of the pairing interaction is neglected (see the next section). 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. The above Hamiltonian can be considerably simplified in the absence of the interband pairing, which is the case if the SO splitting of the bands, E_{SO}, is large compared with all energy scales associated with superconductivity. Since the pairing interaction is effective only inside the shells of width ω_c (the cutoff energy) in the vicinity of the Fermi surfaces, one can set $\lambda_1=\lambda_2=\lambda$ and $\lambda_3=\lambda_4=\lambda'$, and obtain

$$H_{\text{int}} = \frac{1}{2\mathcal{V}}\sum_{\boldsymbol{k}\boldsymbol{k}'\boldsymbol{q}}\sum_{\lambda\lambda'} V_{\lambda\lambda'}(\boldsymbol{k},\boldsymbol{k}')c^\dagger_{\boldsymbol{k}+\boldsymbol{q},\lambda}c^\dagger_{-\boldsymbol{k},\lambda}c_{-\boldsymbol{k}',\lambda'}c_{\boldsymbol{k}'+\boldsymbol{q},\lambda'}, \tag{9}$$

where

$$V_{\lambda\lambda'}(\boldsymbol{k},\boldsymbol{k}') = t_\lambda(\boldsymbol{k})t^*_{\lambda'}(\boldsymbol{k}')\tilde{V}_{\lambda\lambda'}(\boldsymbol{k},\boldsymbol{k}'). \tag{10}$$

The pairing amplitudes $\tilde{V}_{\lambda\lambda'}$ are even in both $\boldsymbol{k}$ and $\boldsymbol{k}'$ (due to the anticommutation of fermionic operators) and also invariant under the point group operations: $\tilde{V}_{\lambda\lambda'}(g^{-1}\boldsymbol{k},g^{-1}\boldsymbol{k}') = \tilde{V}_{\lambda\lambda'}(\boldsymbol{k},\boldsymbol{k}')$.[18]

In the case of large SO band splitting, the order parameter has only intraband components. It is uniform (in the absence of external fields) and can be represented in the form $\Delta_\lambda(\boldsymbol{k})=t_\lambda(\boldsymbol{k})\tilde{\Delta}_\lambda(\boldsymbol{k})$. The gap functions $\tilde{\Delta}_\lambda$ transform according to one of the even irreducible representations of the point group and satisfy the following equations:

$$\tilde{\Delta}_\lambda(\boldsymbol{k}) = -T\sum_n\sum_{\lambda'}\int\frac{d^3\boldsymbol{k}'}{(2\pi)^3}\tilde{V}_{\lambda\lambda'}(\boldsymbol{k},\boldsymbol{k}') \times \frac{\tilde{\Delta}_{\lambda'}(\boldsymbol{k}')}{\omega_n^2 + \xi^2_{\lambda'}(\boldsymbol{k}') + |\tilde{\Delta}_{\lambda'}(\boldsymbol{k}')|^2}. \tag{11}$$

The expression on the right-hand side converges due to the energy cutoff at ω_c.

III. BCS MODEL

Let us calculate the pairing amplitudes and the gap functions in a simple BCS-like model, in which the attractive interaction is both instantaneous in time and local in space:

$$H_{\text{int}} = -V\int d^3\boldsymbol{r}\,\psi^\dagger_\uparrow(\boldsymbol{r})\psi^\dagger_\downarrow(\boldsymbol{r})\psi_\downarrow(\boldsymbol{r})\psi_\uparrow(\boldsymbol{r}) = -\frac{V}{4}\int d^3\boldsymbol{r}(i\sigma_2)_{\alpha\beta}(i\sigma_2)^\dagger_{\gamma\delta}\psi^\dagger_\alpha(\boldsymbol{r})\psi^\dagger_\beta(\boldsymbol{r})\psi_\gamma(\boldsymbol{r})\psi_\delta(\boldsymbol{r}), \tag{12}$$

where $V>0$. Using the band representation of the field operators,

$$\psi_\alpha(\boldsymbol{r}) = \frac{1}{\sqrt{\mathcal{V}}}\sum_{\boldsymbol{k},\lambda}u_{\alpha\lambda}(\boldsymbol{k})e^{i\boldsymbol{k}\boldsymbol{r}}c_{\boldsymbol{k}\lambda}, \tag{13}$$

we obtain the pairing Hamiltonian in the form (8) with

$$V_{\lambda_1\lambda_2\lambda_3\lambda_4}(\boldsymbol{k},\boldsymbol{k}') = -\frac{V}{2}(i\sigma_2)_{\alpha\beta}(i\sigma_2)^{\dagger}_{\gamma\delta}u^{*}_{\alpha\lambda_1}(\boldsymbol{k})u^{*}_{\beta\lambda_2} \times(-\boldsymbol{k})u_{\gamma\lambda_3}(-\boldsymbol{k}')u_{\delta\lambda_4}(\boldsymbol{k}').$$

Here we neglected the difference between $u_{\alpha\lambda}(\pm\boldsymbol{k}+\boldsymbol{q})$ and $u_{\alpha\lambda}(\pm\boldsymbol{k})$, which is $\mathcal{O}(q/k_F)$. In conventional centrosymmetric superconductors, we have $q/k_F \sim (\xi k_F)^{-1} \ll 1$ (ξ is the correlation length). In the noncentrosymmetric case, the above estimate might not work and the $\boldsymbol{q}$ dependence of the pairing interaction might be more important, leading, for instance, to the Lifshitz invariants in the free energy[8,19] and a spatial modulation of the order parameter even in the absence of external fields. We leave this issues to a separate publication.

Using the identities

$$u_{\alpha\lambda}(-\boldsymbol{k}) = t^{*}_{\lambda}(\boldsymbol{k})(i\sigma_2)_{\alpha\beta}u^{*}_{\beta\lambda}(\boldsymbol{k}), \tag{14}$$

and also the unitarity of the matrix $\hat{u}(\boldsymbol{k})$, we obtain for the pairing potential:

$$V_{\lambda_1\lambda_2\lambda_3\lambda_4}(\boldsymbol{k},\boldsymbol{k}') = -\frac{V}{2}t_{\lambda_2}(\boldsymbol{k})t^{*}_{\lambda_3}(\boldsymbol{k}')\delta_{\lambda_1\lambda_2}\delta_{\lambda_3\lambda_4}. \tag{15}$$

Therefore, interband pairing is absent in the BCS model for any strength of the SO coupling. Comparing this expression with Eq. (10), one can see that both the intraband pairing and the pair scattering between the bands are characterized by the same coupling constant: $\tilde{V}_{\lambda\lambda'}(\boldsymbol{k},\boldsymbol{k}') = -V/2$. The pairing symmetry is isotropic, and it follows from Eqs. (11) that the gap functions are the same in both bands: $\tilde{\Delta}_{+}(\boldsymbol{k}) = \tilde{\Delta}_{-}(\boldsymbol{k}) = \eta$. This is not surprising, since the local interaction (12) cannot lead to any $\boldsymbol{k}$ dependence of the gaps.

The critical temperature is given by $T_c = (2e^{\mathbb{C}}/\pi)\omega_c e^{-1/N_F V}$, where $\mathbb{C} \simeq 0.577$ is Euler's constant, $N_F = (N_+ + N_-)/2$, and N_λ is the Fermi-level density of states in the λth band. Although this has the usual BCS form, the superconductivity is non-BCS, because the order parameter resides in two nondegenerate bands, with T_c and η independent of the band splitting and the difference between N_+ and N_-. One can show that both the critical temperature and the gap magnitude are not affected by isotropic scalar impurities.[20]

IV. INTERACTION MEDIATED BY BOSONIC EXCITATIONS

Now we investigate a more general model, in which the pairing is assumed to be due to the exchange of some bosonic excitations. We consider two types of excitations: Scalar (phonons), which couple to the electron density $\rho(\boldsymbol{r}) = \psi^{\dagger}_{\alpha}(\boldsymbol{r})\psi_{\alpha}(\boldsymbol{r})$, and pseudovector (spin fluctuations), which couple to the electron spin density $\boldsymbol{s}(\boldsymbol{r}) = \psi^{\dagger}_{\alpha}(\boldsymbol{r})\boldsymbol{\sigma}_{\alpha\beta}\psi_{\beta}(\boldsymbol{r})$. Using the standard functional-integral representation of the partition function of the system, we obtain the following term in the fermionic action describing an effective two-particle interaction between electrons:

$$S_{\rm int} = \frac{g^2_{\rm ph}}{2}\int dx\,dx'\rho(x)D(x-x')\rho(x') + \frac{g^2_{\rm sf}}{2}\int dx\,dx' s_i(x)\mathcal{D}_{ij}(x-x')s_j(x'), \tag{16}$$

where $x = (\boldsymbol{r},\tau)$ is a shorthand notation for the coordinates in real space and the Matsubara time, $\int dx(\ldots) = \int d\boldsymbol{r}\int_0^\beta d\tau(\ldots)$, $g_{\rm ph}$ and $g_{\rm sf}$ are the coupling constants of electrons with phonons and spin fluctuations, while $D(x-x')$ and $\mathcal{D}_{ij}(x-x')$ are the phonon and spin-fluctuation propagators, respectively. The spin fluctuations can be associated either with the localized spins, if such are present in the system, or with the collective spin excitations of the itinerant electrons (paramagnons).[21] In the latter case, $\mathcal{D}_{ij}(x-x')$ can be expressed in terms of the electron dynamical spin susceptibility $\chi_{ij}(\boldsymbol{q},\omega)$. In general, the interaction (16) is nonlocal both in space and time. The BCS-contact Hamiltonian (12) is recovered when the spin fluctuations are neglected and $g^2_{\rm ph}D(\boldsymbol{r},\tau)$ is replaced by $-V\delta(\boldsymbol{r})\delta(\tau)$.

In the momentum-frequency representation, Eq. (16) yields the following pairing action:

$$S_{\rm int} = \frac{1}{2\Omega}\sum_{kk'q}[g^2_{\rm ph}D(k-k')\delta_{\alpha\delta}\delta_{\beta\gamma} + g^2_{\rm sf}\mathcal{D}_{ij}(k-k')\sigma^i_{\alpha\delta}\sigma^j_{\beta\gamma}] \times \bar{a}_{\alpha}(k+q)\bar{a}_{\beta}(-k)a_{\gamma}(-k')a_{\delta}(k'+q), \tag{17}$$

where $\Omega = \beta\mathcal{V}$ is the space-time volume, $\bar{a}_\alpha(k)$ and $a_\alpha(k)$ are Grassmann fields, $k = (\boldsymbol{k},\omega_n)$, $q = (\boldsymbol{q},\nu_m)$, and $\omega_n = (2n+1)\pi T$ and $\nu_m = 2m\pi T$ are the fermionic and bosonic Matsubara frequencies, respectively. We assume that the conditions of the Migdal theorem are fulfilled, and also neglect the frequency renormalization, which corresponds to the weak-coupling limit of the Eliashberg theory. The theory developed below should work, at least qualitatively, even for such materials as $CePt_3Si$, in which strong electron correlations are responsible for a heavy-fermion behavior and the above assumptions might be inapplicable.

The phonon propagator is real and even in both frequency and momentum, $D(k-k') = D(k'-k)$, and can therefore be written as follows:

$$D(k-k') = D^{g}(k,k') + D^{u}(k,k'), \tag{18}$$

where the first term on the right-hand side, $D^g(k,k') = [D(k-k') + D(k+k')]/2$, is even in both k and k', while the second term, $D^u(k,k') = [D(k-k') - D(k+k')]/2$, is odd in both k and k'.

The spin-fluctuation propagator satisfies $\mathcal{D}_{ij}(k-k') = \mathcal{D}_{ji}(k'-k)$ and can be broken up into the symmetric and antisymmetric in ij parts. Representing the latter in terms of a dual vector $\boldsymbol{R}$, we obtain

$$\mathcal{D}_{ij}(k-k') = \mathcal{D}^{g}_{ij}(k,k') + \mathcal{D}^{u}_{ij}(k,k') + ie_{ijl}R_l(k-k'), \tag{19}$$

where the first (second) term on the right-hand side is an even (odd) function of k and k', while $R_i(k-k') = -R_i(k'-k)$. The antisymmetric component of the spin-fluctuation propagator is associated with the Dzyaloshinskii-Moriya interaction.[22] It is absent in the centrosymmetric case, due to

the additional symmetry $\mathcal{D}_{ij}(k-k')=\mathcal{D}_{ij}(k'-k)$.

After some straightforward algebra (see the Appendix), the action (17) takes the following form:

$$S_{\rm int}=\frac{1}{2\Omega}\sum_{kk'q}V_{\alpha\beta\gamma\delta}(k,k')\bar{a}_\alpha(k+q)\bar{a}_\beta(-k)\times a_\gamma(-k')a_\delta(k'+q), \tag{20}$$

where the pairing interaction is represented as a sum of the k-even, k-odd, and mixed-parity terms: $V=V^g+V^u+V^m$. The even contribution is

$$V^g_{\alpha\beta\gamma\delta}(k,k')=v_g(k,k')(i\sigma_2)_{\alpha\beta}(i\sigma_2)^\dagger_{\gamma\delta}, \tag{21}$$

where

$$v_g(k,k')=\frac{1}{2}[g_{\rm ph}^2D^g(k,k')-g_{\rm sf}^2{\rm tr}\hat{\mathcal{D}}^g(k,k')]. \tag{22}$$

The odd contribution is

$$V^u_{\alpha\beta\gamma\delta}(k,k')=v_{u,ij}(k,k')(i\sigma_i\sigma_2)_{\alpha\beta}(i\sigma_j\sigma_2)^\dagger_{\gamma\delta}, \tag{23}$$

where

$$v_{u,ij}(k,k')=\frac{1}{2}[g_{\rm ph}^2D^u(k,k')+g_{\rm sf}^2{\rm tr}\hat{\mathcal{D}}^u(k,k')]\delta_{ij}-g_{\rm sf}^2\mathcal{D}^u_{ij}(k,k'). \tag{24}$$

Finally, the mixed-parity contribution is

$$V^m_{\alpha\beta\gamma\delta}(k,k')=v_{m,i}(k,k')(i\sigma_i\sigma_2)_{\alpha\beta}(i\sigma_2)^\dagger_{\gamma\delta}+v_{m,i}(k',k)\times(i\sigma_2)_{\alpha\beta}(i\sigma_i\sigma_2)^\dagger_{\gamma\delta}, \tag{25}$$

where

$$v_{m,i}(k,k')=\frac{g_{\rm sf}^2}{2}[R_i(k-k')+R_i(k+k')]. \tag{26}$$

The first term on the right-hand side of Eq. (25) is odd in k and even in k', while the second term is even in k and odd in k'.

We would like to note that expressions (21), (23), and (25) have completely general form in the sense that they do not rely on our assumptions about boson-mediated interactions and exhaust all possible spin structures of the pairing amplitude. Under the point group operations g, the coefficients v_g, $v_{u,ij}$, and $\boldsymbol{v}_m$ transform like a scalar, a second-rank tensor, and a pseudovector, respectively, and satisfy the invariance conditions $v_g(g^{-1}\boldsymbol{k},\omega_n;g^{-1}\boldsymbol{k}',\omega_{n'})=v_g(\boldsymbol{k},\omega_n;\boldsymbol{k}',\omega_{n'})$, etc. By analogy with the theory of superconductivity in centrosymmetric compounds, see, e.g., Ref. 24, Eqs. (21) and (23) correspond to spin-singlet and spin-triplet pairing channels respectively, while Eq. (25) describes singlet-triplet mixing. The possibility of singlet-triplet mixing due to the Dzyaloshinskii-Moriya interaction in the static case was pointed out in Ref. 23.

Next, we use Eqs. (2) to transform the pairing action into the band representation. Using identities (14), we obtain the transformation rules for the pair creation operators in the spin-singlet and spin-triplet channels

$$(i\sigma_2)_{\alpha\beta}\bar{a}_\alpha(k+q)\bar{a}_\beta(-k)=-\sum_{\lambda_{1,2}}t_{\lambda_2}(\boldsymbol{k})\delta_{\lambda_1\lambda_2}\bar{c}_{\lambda_1}(k+q)\bar{c}_{\lambda_2}(-k),$$

$$(i\boldsymbol{\sigma}\sigma_2)_{\alpha\beta}\bar{a}_\alpha(k+q)\bar{a}_\beta(-k)=-\sum_{\lambda_{1,2}}t_{\lambda_2}(\boldsymbol{k})\boldsymbol{\tau}_{\lambda_1\lambda_2}(\boldsymbol{k})\times\bar{c}_{\lambda_1}(k+q)\bar{c}_{\lambda_2}(-k),$$

where

$$\hat{\tau}_i(\boldsymbol{k})=\hat{u}^\dagger(\boldsymbol{k})\hat{\sigma}_i\hat{u}(\boldsymbol{k}). \tag{27}$$

Inserting these in Eq. (20), we obtain

$$S_{\rm int}=\frac{1}{2\Omega}\sum_{kk'q}\sum_{\lambda_{1,2,3,4}}V_{\lambda_1\lambda_2\lambda_3\lambda_4}(k,k')\times\bar{c}_{\lambda_1}(k+q)\bar{c}_{\lambda_2}(-k)c_{\lambda_3}(-k')c_{\lambda_4}(k'+q), \tag{28}$$

where

$$V_{\lambda_1\lambda_2\lambda_3\lambda_4}(k,k')=t_{\lambda_2}(\boldsymbol{k})t^*_{\lambda_3}(\boldsymbol{k}')\tilde{V}_{\lambda_1\lambda_2\lambda_3\lambda_4}(k,k'), \tag{29}$$

and

$$\begin{aligned}\tilde{V}_{\lambda_1\lambda_2\lambda_3\lambda_4}(k,k')=&\,v_g(k,k')\delta_{\lambda_1\lambda_2}\delta_{\lambda_3\lambda_4}\\&+v_{u,ij}(k,k')\tau_{i,\lambda_1\lambda_2}(\boldsymbol{k})\tau_{j,\lambda_3\lambda_4}(\boldsymbol{k}')\\&+v_{m,i}(k,k')\tau_{i,\lambda_1\lambda_2}(\boldsymbol{k})\delta_{\lambda_3\lambda_4}\\&+v_{m,i}(k',k)\delta_{\lambda_1\lambda_2}\tau_{i,\lambda_3\lambda_4}(\boldsymbol{k}').\end{aligned} \tag{30}$$

The pairing amplitudes satisfy the following symmetry properties:

$$\tilde{V}_{\lambda_2\lambda_1\lambda_3\lambda_4}(-k,k')=\lambda_1\lambda_2\tilde{V}_{\lambda_1\lambda_2\lambda_3\lambda_4}(k,k'),$$

$$\tilde{V}_{\lambda_1\lambda_2\lambda_4\lambda_3}(k,-k')=\lambda_3\lambda_4\tilde{V}_{\lambda_1\lambda_2\lambda_3\lambda_4}(k,k').$$

To obtain these, we used the anticommutation of the Grassmann fields in Eq. (28) and also the expressions (4) for the phase factors in Eq. (29).

It follows from Eq. (30) that, in general, all possible channels are present in the pairing interaction, including interband pairing. The latter is absent, for any magnitude of the SO band splitting, if the odd harmonics of the bosonic propagators are negligible, so that $v_{u,ij}(k,k')=0$ and $v_{m,i}(k,k')=0$. This happens, in particular, for a fully isotropic interaction, in which case $v_g(k,k')=v_g(\omega_n,\omega_{n'})$.

We are particularly interested in the limit of large SO band splitting, which is relevant for the majority of noncentrosymmetric superconducting materials. In this limit, we set $\lambda_1=\lambda_2=\lambda$ and $\lambda_3=\lambda_4=\lambda'$ in Eq. (30) (the case of arbitrary band splitting, with both intra- and interband components of the order parameter present, will be considered in a separate publication). Since $\boldsymbol{\tau}_{\lambda\lambda}=\lambda\hat{\boldsymbol{\gamma}}(\boldsymbol{k})$, the pairing action becomes

$$S_{\rm int} = \frac{1}{2\Omega}\sum_{kk'q}\sum_{\lambda\lambda'} t_\lambda(\boldsymbol{k}) t^*_{\lambda'}(\boldsymbol{k}')\tilde{V}_{\lambda\lambda'}(k,k') \times \bar{c}_\lambda(k+q)\bar{c}_\lambda(-k)c_{\lambda'}(-k')c_{\lambda'}(k'+q), \quad (31)$$

where

$$\tilde{V}_{\lambda\lambda'}(k,k') = v_g(k,k') + \lambda\lambda' v_{u,ij}(k,k')\hat{\gamma}_i(\boldsymbol{k})\hat{\gamma}_j(\boldsymbol{k}') + \lambda \boldsymbol{v}_m(k,k')\hat{\boldsymbol{\gamma}}(\boldsymbol{k}) + \lambda' \boldsymbol{v}_m(k',k)\hat{\boldsymbol{\gamma}}(\boldsymbol{k}'). \quad (32)$$

This expression, together with Eqs. (22), (24), and (26) relates the amplitudes of the intraband pairing and the interband pair scattering to the bosonic excitation spectra. Note that $\tilde{V}_{\lambda\lambda'}(k,k')$ is even in both k and k'. Treating the interaction (31) in the mean-field approximation, see, e.g., Ref. 24, one introduces the order parameters $\Delta_\lambda(k) = t_\lambda(\boldsymbol{k})\tilde{\Delta}_\lambda(\boldsymbol{k},\omega_n)$, where, due to the symmetry of the pairing amplitudes, $\tilde{\Delta}_\lambda(-\boldsymbol{k},-\omega_n) = \tilde{\Delta}_\lambda(\boldsymbol{k},\omega_n)$.

A. Weak coupling model

In order to make progress, we approximate the frequency dependence of the pairing amplitudes by an anisotropic "square-well" model:[25]

$$\tilde{V}_{\lambda\lambda'}(k,k') = \tilde{V}_{\lambda\lambda'}(\boldsymbol{k},\boldsymbol{k}')\theta(\omega_c - |\omega_n|)\theta(\omega_c - |\omega_{n'}|), \quad (33)$$

where $\theta(x)$ is the step function, ω_c is the frequency cutoff, and $\tilde{V}_{\lambda\lambda'}(\boldsymbol{k},\boldsymbol{k}')$ depend on the directions of $\boldsymbol{k}$ and $\boldsymbol{k}'$ near the corresponding Fermi surfaces. The approximation (33) has been used both for conventional phononic pairing interaction [see Ref. 25], and also for spin-fluctuation mediated interaction [see Ref. 26]. The "square-well" decomposition also holds for the gap functions: $\tilde{\Delta}_\lambda(\boldsymbol{k},\omega_n) = \tilde{\Delta}_\lambda(\boldsymbol{k})\theta(\omega_c - |\omega_n|)$, so that the energy of quasiparticle excitations in the λth band is given by

$$E_\lambda(\boldsymbol{k}) = \sqrt{\xi^2_\lambda(\boldsymbol{k}) + |\tilde{\Delta}_\lambda(\boldsymbol{k})|^2}. \quad (34)$$

The gap functions satisfy Eqs. (11), in which the Matsubara sum is cut off at ω_c.

The pairing amplitude given by the matrix Eq. (32) is invariant under all operations from the crystal point group $\mathbb{G}$, therefore $\tilde{V}_{\lambda\lambda'}(g^{-1}\boldsymbol{k}, g^{-1}\boldsymbol{k}') = \tilde{V}_{\lambda\lambda'}(\boldsymbol{k},\boldsymbol{k}')$. Therefore, the momentum dependence of each matrix element can be represented as a sum of the products of the basis functions of irreducible representations of $\mathbb{G}$. In general, the basis functions are different for each matrix element. Neglecting this complication the pairing amplitude can be factorized as follows:

$$\tilde{V}_{\lambda\lambda'}(\boldsymbol{k},\boldsymbol{k}') = -\sum_a V^a_{\lambda\lambda'}\sum_{i=1}^{d_a}\phi_{a,i}(\boldsymbol{k})\phi^*_{a,i}(\boldsymbol{k}'), \quad (35)$$

where a labels the irreducible representations (of dimensionality d_a) of $\mathbb{G}$, which correspond to pairing channels of different symmetry, with $\phi_{a,i}(\boldsymbol{k})$ being the even basis functions.[24] The coupling constants $V^a_{\lambda\lambda'}$ form a Hermitian matrix, which becomes real symmetric if the basis functions are real. Keeping only the irreducible representation Γ which corresponds to the maximum critical temperature, the gap functions take the form

$$\tilde{\Delta}_\lambda(\boldsymbol{k}) = \sum_{i=1}^{d_\Gamma}\eta_{\lambda,i}\phi_i(\boldsymbol{k}), \quad (36)$$

and $\eta_{\lambda,i}$ are the superconducting order parameter components in the λth band. The basis functions are assumed to satisfy the following orthogonality conditions: $\langle\phi^*_i(\boldsymbol{k})\phi_j(\boldsymbol{k})\rangle_\lambda = \delta_{ij}$, where the angular brackets denote the averaging over the λth Fermi surface.

Linearizing the gap equations (11) we obtain the following expression for the critical temperature:

$$T_c = \frac{2e^{\mathbb{C}}}{\pi}\omega_c e^{-1/g}, \quad (37)$$

where

$$g = \frac{g_{++}+g_{--}}{2} + \sqrt{\left(\frac{g_{++}-g_{--}}{2}\right)^2 + g_{+-}g_{-+}} \quad (38)$$

is the effective coupling constant, and

$$g_{\lambda\lambda'} = V_{\lambda\lambda'}N_{\lambda'}. \quad (39)$$

While the critical temperature is the same for all d_Γ components of $\boldsymbol{\eta}_\lambda$, the gap structure in the superconducting state below T_c, see Eq. (36), is determined by the nonlinear terms in the free energy, which essentially depend on the symmetry of the dominant pairing channel.

V. PAIRING SYMMETRY IN A CUBIC CRYSTAL

In the case of isotropic pairing interaction, one can write $v_g(k,k') = v_g(\omega_n,\omega_{n'}) = -V_g\theta(\omega_c - |\omega_n|)\theta(\omega_c - |\omega_{n'}|)$ in the square-well approximation. In this way, one recovers the BCS model of Sec. III, with $V = 2V_g$ and the same isotropic gaps in both bands.

To illustrate the effects of the interaction anisotropy on the gap structure, let us consider the following example. In a cubic crystal with $\mathbb{G} = \mathbf{O}$, the SO coupling can be described by $\boldsymbol{\gamma}(\boldsymbol{k}) = \gamma_0\boldsymbol{k}$. This model is applicable to the $Li_2(Pd_{1-x},Pt_x)_3B$ family of noncentrosymmetric compounds. The attractive interaction in these materials is likely mediated by phonons,[9,27] therefore we neglect spin fluctuations by setting $g_{\rm sf} = 0$ in expressions (22), (24), and (26). Then, $v_g(k,k') = (g^2_{\rm ph}/2)D^g(k,k')$, $v_{u,ij}(k,k') = (g^2_{\rm ph}/2)D^u(k,k')\delta_{ij}$, and $v_{m,i}(k,k') = 0$. Using the square-well approximation, one has

$$v_g(k,k') = v_g(\boldsymbol{k},\boldsymbol{k}')\,\theta(\omega_c - |\omega_n|)\,\theta(\omega_c - |\omega_{n'}|),$$

$$v_{u,ij}(k,k') = v_{u,ij}(\boldsymbol{k},\boldsymbol{k}')\,\theta(\omega_c - |\omega_n|)\,\theta(\omega_c - |\omega_{n'}|),$$

with the momentum dependence inherited from the phonon propagator. Assuming a spherical Fermi surface and keeping only the s and p harmonics in the phonon propagator, we obtain

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

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

$$v_{m,i}(\boldsymbol{k},\boldsymbol{k}') = 0, \tag{40}$$

where V_g and V_u are constants. Note that this interaction is the same as the one considered phenomenologically by Edelstein in Ref. 14. From Eq. (32) we obtain the pairing amplitudes in the band representation as follows:

$$\tilde{V}_{\lambda\lambda'}(\boldsymbol{k},\boldsymbol{k}') = -V_g - \lambda\lambda' V_u(\hat{\boldsymbol{k}}\hat{\boldsymbol{k}}')^2. \tag{41}$$

The components of the symmetric tensor $\hat{k}_i\hat{k}_j$ transform according to the representation A_1+E+F_2, where A_1, E, and F_2 are respectively one-, two-, and three-dimensional irreducible representations of the cubic group $\boldsymbol{O}$ (the notations are the same as in Ref. 28). Therefore there are three pairing channels in the expansion (35), with the following basis functions and coupling constants:

$$V^{A_1}_{\lambda\lambda'} = V_g + \frac{1}{3}\lambda\lambda' V_u, \quad \phi_{A_1}(\boldsymbol{k}) = 1,$$

$$V^{E}_{\lambda\lambda'} = \frac{2}{15}\lambda\lambda' V_u,\ \phi_E(\boldsymbol{k}) \propto (\hat{k}_x^2 + \omega\hat{k}_y^2 + \omega^*\hat{k}_z^2, \hat{k}_x^2 + \omega^*\hat{k}_y^2 + \omega\hat{k}_z^2),$$

$$V^{F_2}_{\lambda\lambda'} = \frac{2}{15}\lambda\lambda' V_u,\ \phi_{F_2}(\boldsymbol{k}) \propto (\hat{k}_y\hat{k}_z, \hat{k}_z\hat{k}_x, \hat{k}_x\hat{k}_y), \tag{42}$$

where $\omega = \exp(2\pi i/3)$.

Since phonons typically lead to a local attraction and cannot give rise to a substantial $\boldsymbol{k}$ dependence of the interaction, we expect that the A_1 pairing channel dominates. Then the gap functions in the two bands [Eqs. (36)] are isotropic: $\tilde{\Delta}_\lambda(\boldsymbol{k}) = \eta_\lambda$, and satisfy the equations

$$\eta_\lambda = \sum_{\lambda'} g_{\lambda\lambda'}\pi T \sum_n \frac{\eta_{\lambda'}}{\sqrt{\omega_n^2 + \eta_{\lambda'}^2}}, \tag{43}$$

where $g_{\lambda\lambda'} = V^{A_1}_{\lambda\lambda'} N_{\lambda'}$. The critical temperature is given by Eq. (37). The gap magnitudes are not necessarily equal: For instance, in the vicinity of T_c we find the following expression for the gap variation between the bands:

$$r \equiv \frac{\eta_+ - \eta_-}{\eta_+ + \eta-} = \frac{g_{++} - g_{--} - 2g_{-+} + \sqrt{\mathcal{D}}}{g_{++} - g_{--} + 2g_{-+} + \sqrt{\mathcal{D}}}, \tag{44}$$

where $\mathcal{D} = \sqrt{(g_{++} - g_{--})^2 + 4g_{+-}g_{-+}}$. Assuming that $N_+ - N_-$ is small and that $V_g \gg V_u$, we have

$$r \simeq \frac{V_u}{6V_g}\frac{N_+ - N_-}{N_F}. \tag{45}$$

Thus the gaps are different only if an appreciable p-wave harmonic is present in the phonon-mediated interaction *and* the SO coupling is sufficiently strong to create a considerable difference between the densities of states in the two bands.

The coupling strengths being the same in both bands is not a generic situation. In the spirit of the standard model of two-band superconductivity,[13] it is possible that the coupling constants corresponding to the intraband pairing channels and the interband pair scattering are all different. To obtain this we consider a generalization of the model (40) which includes, along with phonons, also a contribution from spin fluctuations. In the absence of detailed information about the phonon and spin-fluctuation spectra in real noncentrosymmetric materials, in particular in $Li_2(Pd_{1-x},Pt_x)_3B$, we use the model which includes only the lowest angular harmonics consistent with the symmetry requirements:

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

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

$$v_{m,i}(\boldsymbol{k},\boldsymbol{k}') = -V_m\hat{k}_i. \tag{46}$$

Here the coefficients V_g and V_u are, in general, different from those in the model (40). In the band representation, the pairing amplitudes become

$$\tilde{V}_{\lambda\lambda'}(\boldsymbol{k},\boldsymbol{k}') = -V_g - \lambda\lambda'[V_u(\hat{\boldsymbol{k}}\hat{\boldsymbol{k}}')^2 + V_u'] - (\lambda+\lambda')V_m. \tag{47}$$

There are three pairing channels, corresponding to the A_1, E, and F_2 representations; see Eqs. (42). The coupling constants in the A_1 channel now have the following form:

$$V^{A_1}_{\lambda\lambda'} = V_g + \frac{1}{3}\lambda\lambda' V_u + \lambda\lambda' V_u' + (\lambda+\lambda')V_m. \tag{48}$$

The gap functions are isotropic: $\tilde{\Delta}_\lambda(\boldsymbol{k}) = \eta_\lambda$, where the η_λs are found from Eqs. (43). The difference from the previous case is that now $\eta_+ \neq \eta_-$ even if the density of states variation between the bands is negligible, i.e., $N_+ = N_- = N_F$. Assuming that V_m is smaller than the other constants (i.e., the singlet-triplet mixing due to the Dzyaloshinskii-Moriya interaction is weak), we obtain from Eq. (44) that

$$r \simeq \frac{V_m}{V_g - V_u/3 - V_u'} \tag{49}$$

near the critical temperature.

Finally let us consider the case of p-wave interaction dominating, which leads to an anisotropic pairing of the F_2 symmetry. This happens if V_u is large enough, and the degeneracy between the F_2 and E channels is lifted, e.g., by the Fermi surface anisotropy. The order parameter has the following form:

$$\tilde{\Delta}_\lambda(\boldsymbol{k}) = \lambda(\eta_1 \hat{k}_y \hat{k}_z + \eta_2 \hat{k}_z \hat{k}_x + \eta_3 \hat{k}_x \hat{k}_y). \tag{50}$$

The symmetry of the gap, in particular the location of the nodes, depends on the relation between the components of $\boldsymbol{\eta}$. There are four stable states of a three-dimensional order parameter in a cubic crystal:[29] (i) $\boldsymbol{\eta}=\eta_0(1,0,0)$, with two lines of nodes at $k_z=0$ and $k_y=0$; (ii) $\boldsymbol{\eta}=\eta_0(1,i,0)$, with a line of nodes at $k_z=0$, and also point nodes at $k_x=k_y=0$; (iii) $\boldsymbol{\eta}=\eta_0(1,1,1)$, with two lines of nodes at the intersection of the planes $\hat{k}_x+\hat{k}_y+\hat{k}_z=\pm 1$ with the Fermi surface, and also point nodes at $k_x=k_y=0$, $k_y=k_z=0$, and $k_z=k_x=0$; and (iv) $\boldsymbol{\eta}=\eta_0(1,\omega,\omega^2)$, with point nodes at $k_x=k_y=0$, $k_y=k_z=0$, $k_z=k_x=0$, and $k_x=k_y=k_z$. For the first three states one would have $c_V(T)\propto T^2$ at low temperatures,[30] while for the last one $c_V(T)\propto T^3$.

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

$$\Delta_{\alpha\beta}(\boldsymbol{k}) = \psi(\boldsymbol{k})(i\hat{\sigma}_2)_{\alpha\beta} + \boldsymbol{d}(\boldsymbol{k})(i\hat{\boldsymbol{\sigma}}\hat{\sigma}_2)_{\alpha\beta}, \tag{51}$$

where

$$\psi(\boldsymbol{k}) = -\frac{\tilde{\Delta}_+(\boldsymbol{k}) + \tilde{\Delta}_-(\boldsymbol{k})}{2} \tag{52}$$

is the spin-singlet component, and

$$\boldsymbol{d}(\boldsymbol{k}) = -\frac{\tilde{\Delta}_+(\boldsymbol{k}) - \tilde{\Delta}_-(\boldsymbol{k})}{2}\hat{\boldsymbol{\gamma}}(\boldsymbol{k}) \tag{53}$$

is the spin-triplet component.[12,31] The relative strength of the triplet and singlet order parameters is controlled by the difference between η_+ and η_-: $|\boldsymbol{d}|/|\psi|=r$; see Eq. (44). In agreement with Ref. 15, only the component of $\boldsymbol{d}(\boldsymbol{k})$ which is parallel to $\hat{\boldsymbol{\gamma}}(\boldsymbol{k})$ survives (is "protected") in the limit of large SO band splitting. However, in the case of a weakly anisotropic phonon-dominated interaction, it follows from expression (45) that the triplet component is negligibly small. In the opposite case, when the interaction is strongest in the p-wave channel, one obtains from Eq. (42) that $\psi(\boldsymbol{k})=0$, i.e., the pairing is purely triplet.

VI. CONCLUSIONS AND DISCUSSION

We have studied the pairing symmetry in noncentrosymmetric superconductors with SO splitting of the electron bands. The pairing interaction is derived using a microscopic model which includes both phonons and spin fluctuations. The interband pairing is shown to be absent for any strength of the SO coupling, if the interaction anisotropy is negligible. We have analyzed possible gap structures in the strong SO coupling limit with only intraband pairing and interband pair scattering present, using a cubic system as an example. If phonons are dominant, then the superconducting gaps in both bands are isotropic and nodeless (barring accidental zeros of the basis function of the unity representation), but do not necessarily have the same magnitude.

Let us discuss the application of our results to the noncentrosymmetric compounds $Li_2(Pd_{1-x},Pt_x)_3B$, where x ranges from 0 to 1 (Ref. 6). The critical temperature varies from 7–8 K for $x=0$ to 2.2–2.8 K for $x=1$. The electronic band structure also exhibits considerable variation: The SO band splitting in Li_2Pd_3B is as large as 30 meV, while in Li_2Pt_3B it reaches 200 meV (Ref. 9), which in both cases is much larger than T_c. Due to the absence of strong correlation effects and magnetic order, these materials provide a convenient testing ground for theories of noncentrosymmetric superconductivity. Superconducting pairing in Li_2Pd_3B is due to the exchange of phonons, and the monotonic, almost linear, dependence of T_c on the doping level x (Ref. 6) suggests that it remains phononic for all x from 0 to 1.[9,27]

Experimental data on the magnetic penetration depth,[32] the electronic specific heat,[33] and the NMR characteristics,[34] all seem to agree that Li_2Pd_3B is a conventional BCS-like superconductor with no gap nodes. In contrast, the gap structure in Li_2Pt_3B is still a subject of intensive debates. While earlier experiments, see Refs. [32–34], suggested the presence of lines of nodes in the gap, the recent μSR and specific heat data[35] have found no evidence of those. Moreover, according to Ref. 35, the whole $Li_2(Pd_{1-x},Pt_x)_3B$ family of compounds are single-gap isotropic superconductors. This conclusion is consistent with our results, see Sec. V. Indeed, assuming that the pairing interaction in $Li_2(Pd_{1-x},Pt_x)_3B$ is phononic and therefore only weakly anisotropic for all x, we obtain that the A_1 channel always dominates, giving rise to nodeless isotropic gaps of essentially equal magnitudes in both bands. In order to create a noticeable difference between the gap magnitudes, see Eq. (45), the interaction anisotropy would have to be very strong: Since $(N_+-N_-)/N_F \sim E_{SO}/\epsilon_F$ and varies from 0.03 in Li_2Pd_3B to 0.2 in Li_2Pt_3B, the strength of the p-wave harmonic must be at least an order of magnitude larger than that of the s-wave harmonic, which is highly unlikely for a phonon-mediated interaction.

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APPENDIX: DERIVATION OF EQS. (21)–(26)

Let us start from Eq. (17), in which we substitute expressions (18) and (19):

$$S_{\text{int}} = \frac{1}{2\Omega}\sum_{kk'q}\{g_{\text{ph}}^2[D^g(k,k')+D^u(k,k')]\delta_{\alpha\delta}\delta_{\beta\gamma} + g_{\text{sf}}^2[\mathcal{D}_{ij}^g(k,k') + \mathcal{D}_{ij}^u(k,k') + ie_{ijl}R_l(k-k')]\sigma_{\alpha\delta}^i\sigma_{\beta\gamma}^j\} \times \bar{a}_\alpha(k+q)\bar{a}_\beta(-k)a_\gamma(-k')a_\delta(k'+q). \tag{A1}$$

The q dependence of the fermionic fields plays no role in the algebraic transformations below; hence we use a shorter expression on the right-hand side:

$$S_{\text{int}} \to \frac{1}{2\Omega}(I^g + I^u + I^m), \tag{A2}$$

where

$$I^g = \frac{1}{4}\sum_{kk'} [g_{\rm ph}^2 D^g(k,k')\delta_{\alpha\delta}\delta_{\beta\gamma} + g_{\rm sf}^2 \mathcal{D}_{ij}^g(k,k')\sigma_{\alpha\delta}^i\sigma_{\beta\gamma}^j]$$
$$\times [\bar{a}_\alpha(k)\bar{a}_\beta(-k) - \bar{a}_\beta(k)\bar{a}_\alpha(-k)]$$
$$\times [a_\gamma(-k')a_\delta(k') - a_\delta(-k')a_\gamma(k')],$$

$$I^u = \frac{1}{4}\sum_{kk'} [g_{\rm ph}^2 D^u(k,k')\delta_{\alpha\delta}\delta_{\beta\gamma} + g_{\rm sf}^2 \mathcal{D}_{ij}^u(k,k')\sigma_{\alpha\delta}^i\sigma_{\beta\gamma}^j]$$
$$\times [\bar{a}_\alpha(k)\bar{a}_\beta(-k) + \bar{a}_\beta(k)\bar{a}_\alpha(-k)] \times [a_\gamma(-k')a_\delta(k')$$
$$+ a_\delta(-k')a_\gamma(k')],$$

$$I^m = \frac{1}{8} ie_{ijl} g_{\rm sf}^2 \sum_{kk'} [R_l(k-k') + R_l(k+k')]\sigma_{\alpha\delta}^i\sigma_{\beta\gamma}^j]$$
$$\times [\bar{a}_\alpha(k)\bar{a}_\beta(-k) + \bar{a}_\beta(k)\bar{a}_\alpha(-k)] \times [a_\gamma(-k')a_\delta(k')$$
$$- a_\delta(-k')a_\gamma(k')] + \frac{1}{8} ie_{ijl} g_{\rm sf}^2 \sum_{kk'} [R_l(k-k')$$
$$- R_l(k+k')]\sigma_{\alpha\delta}^i\sigma_{\beta\gamma}^j] \times [\bar{a}_\alpha(k)\bar{a}_\beta(-k) - \bar{a}_\beta(k)\bar{a}_\alpha(-k)]$$
$$\times [a_\gamma(-k')a_\delta(k') + a_\delta(-k')a_\gamma(k')].$$

The even in k combinations of the fermionic fields can be represented as follows:

$$\bar{a}_\alpha(k)\bar{a}_\beta(-k) - \bar{a}_\beta(k)\bar{a}_\alpha(-k)$$
$$= -(i\sigma_2)_{\alpha\beta}^\dagger (i\sigma_2)_{\mu\nu}\bar{a}_\mu(k)\bar{a}_\nu(-k),$$

$$a_\gamma(-k')a_\delta(k') - a_\delta(-k')a_\gamma(k')$$
$$= -(i\sigma_2)_{\gamma\delta}(i\sigma_2)_{\rho\sigma}^\dagger a_\rho(-k')a_\sigma(k'), \quad \text{(A3)}$$

while the odd combinations have the form

$$\bar{a}_\alpha(k)\bar{a}_\beta(-k) + \bar{a}_\beta(k)\bar{a}_\alpha(-k)$$
$$= (i\sigma_i\sigma_2)_{\alpha\beta}^\dagger (i\sigma_i\sigma_2)_{\mu\nu}\bar{a}_\mu(k)\bar{a}_\nu(-k),$$

$$a_\gamma(-k')a_\delta(k') + a_\delta(-k')a_\gamma(k')$$
$$= (i\sigma_i\sigma_2)_{\gamma\delta}(i\sigma_i\sigma_2)_{\rho\sigma}^\dagger a_\rho(-k')a_\sigma(k'). \quad \text{(A4)}$$

Using the matrix identities

$$\delta_{\alpha\delta}\delta_{\beta\gamma}(i\sigma_2)_{\alpha\beta}^\dagger (i\sigma_2)_{\gamma\delta} = 2,$$

$$(\sigma_i)_{\alpha\delta}(\sigma_j)_{\beta\gamma}(i\sigma_2)_{\alpha\beta}^\dagger (i\sigma_2)_{\gamma\delta} = -2\delta_{ij},$$

$$\delta_{\alpha\delta}\delta_{\beta\gamma}(i\sigma_i\sigma_2)_{\alpha\beta}^\dagger (i\sigma_j\sigma_2)_{\gamma\delta} = 2\delta_{ij},$$

$$(\sigma_i)_{\alpha\delta}(\sigma_j)_{\beta\gamma}(i\sigma_m\sigma_2)_{\alpha\beta}^\dagger (i\sigma_n\sigma_2)_{\gamma\delta} = 2(\delta_{ij}\delta_{mn} - \delta_{im}\delta_{jn} - \delta_{in}\delta_{jm}),$$

$$(\sigma_i)_{\alpha\delta}(\sigma_j)_{\beta\gamma}(i\sigma_m\sigma_2)_{\alpha\beta}^\dagger (i\sigma_2)_{\gamma\delta} = 2ie_{ijm},$$

$$(\sigma_i)_{\alpha\delta}(\sigma_j)_{\beta\gamma}(i\sigma_2)_{\alpha\beta}^\dagger (i\sigma_m\sigma_2)_{\gamma\delta} = -2ie_{ijm}, \quad \text{(A5)}$$

we arrive at Eqs. (21)–(26).

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