

Spin-Orbit Locking as a Protection Mechanism of the Odd-Parity Superconducting State against Disorder

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Unconventional superconductors host a plethora of interesting physical phenomena. However, the standard theory of superconductors suggests that unconventional pairing is highly sensitive to disorder, and hence can only be observed in ultraclean systems. We find that due to an emergent chiral symmetry, spin-orbital locking can parametrically suppress pair decoherence introduced by impurity scattering in odd-parity superconductors. Our work demonstrates that disorder is not an obstacle to realize odd-parity superconductivity in materials with strong spin-orbit coupling.

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The quest for topological superconductors [1–5] is an exciting research area in condensed matter physics. A necessary condition for topological superconductors is unconventional pairing symmetry. Based on an earlier parity criterion [6], it has been shown that under fairly general conditions, time-reversal-invariant topological superconductivity is realized if the pairing symmetry is odd under spatial inversion [7,8]. Such odd-parity pairing occurs in the Ballian-Werthamer phase of superfluid helium-3 [9], and likely in certain heavy fermion superconductors [10,11].

A recent theoretical study [7] suggests that doped narrow-gap semiconductors are candidates for odd-parity topological superconductors. Here the strong spin-orbital coupling in the band structure favors a novel interorbital, odd-parity pairing, even when the mechanism for superconductivity is conventional electron-phonon interaction. Experimentally, several materials in this class, including Cu-doped Bi₂Se₃ [12], Tl-doped PbTe [13], and In-doped SnTe [14], exhibit superconductivity with unusually high transition temperatures (2–4 K) relative to their low carrier densities ($\sim 10^{20}$ cm⁻³). Recently, some evidence of non *s*-wave pairing in Cu_xBi₂Se₃ has been reported [15–17], including the presence of a zero-bias conductance peak in point-contact spectroscopy [18,19].

An important issue in the study of unconventional superconductors is their robustness against disorder. Within the Bardeen-Cooper-Schrieffer theory, *s*-wave pairing is immune to nonmagnetic impurities [20], while other pairing symmetries are more fragile [21]. For instance, the transition temperature of Sr₂RuO₄ that is believed to be a spin-triplet superconductor is strongly suppressed by disorder [22]. This seems to be a major obstacle for realizing odd-parity superconductivity in doped narrow-gap semiconductors.

In this Letter, we study the effect of disorder on the proposed odd-parity superconducting state in narrow-gap semiconductors [7,23]. We mostly focus on scalar impurities which are usually the most common type of

disorder. Such an isotropic scattering potential arises from Coulomb interactions between the electrons and lattice defects. Contrary to conventional wisdom, we find that the destructive pair-breaking effect of disorder is dramatically suppressed by an approximate chiral symmetry in the spin-orbital locked band structure. In view of our study, the prospect of topological superconductivity in narrow-gap semiconductors appears brighter than before.

For concreteness, we start our analysis with the following noninteracting four band $\mathbf{k} \cdot \mathbf{p}$ Hamiltonian:

$$H_0(\mathbf{k}) = \psi^\dagger(\mathbf{k})[m\sigma_x + v\sigma_z(k_x s_y - k_y s_x) + v_z k_z \sigma_y]\psi(\mathbf{k}). \quad (1)$$

H_0 has the form of a massive Dirac Hamiltonian. Here, v and v_z are the velocities of the electrons in the *x*-*y* plane and *z* direction, respectively, while the Dirac mass m (not to be confused with the effective mass) determines the energy gap between the bands. Equation (1) describes the band structure of a broad class of narrow-gap semiconductors with inversion symmetry near time-reversal-invariant momenta [6]. For example, in the context of doped Bi₂Se₃, PbTe, and SnTe, s_i are Pauli matrices in spin space, and σ_i are Pauli matrices associated with the orbital degrees of freedom [23,24]. Specifically for doped Bi₂Se₃, we use $\sigma_z = \pm 1$ to label the two p_z -like orbitals located at the upper and lower part of the quintuple layer unit cell. The two orbitals (+ and -) transform into each other under spatial inversion with respect to the center of the unit cell.

Short range (phonon mediated) attractive interactions can generate pairing with two distinct symmetries. One is the conventional spin-singlet intraorbital state, while the other is the unconventional spin-triplet, orbital singlet paired state [7]:

$$\Delta_1(\mathbf{k}) \propto \sum_{\sigma=\pm} \langle \psi_{\sigma,\uparrow}(\mathbf{k}) \psi_{\sigma,\downarrow}(-\mathbf{k}) - \psi_{\sigma,\downarrow}(\mathbf{k}) \psi_{\sigma,\uparrow}(-\mathbf{k}) \rangle; \quad (2a)$$

$$\Delta_2(\mathbf{k}) \propto \sum_{\sigma=\pm} \sigma \langle \psi_{\sigma,\uparrow}(\mathbf{k}) \psi_{-\sigma,\downarrow}(-\mathbf{k}) + \psi_{\sigma,\downarrow}(\mathbf{k}) \psi_{-\sigma,\uparrow}(-\mathbf{k}) \rangle. \quad (2b)$$

The Δ_1 pairing is invariant under all symmetry operations of the D_{3d} point group (*s*-wave), whereas Δ_2 is odd under spatial inversion (which interchanges the two orbitals) and belongs to the A_{1u} representation. In Ref. [7] it has been shown that, in the absence of disorder, the strength of the interorbital and intraorbital attractive interaction determines which pairing susceptibility diverges more strongly. Here, we examine the effect of disorder on the odd-parity pairing assuming the interaction favors this state. In contrast to the well known *p*-wave spin-triplet superconductivity, here the Δ_2 order parameter is independent of momentum, but has a nontrivial internal structure in orbital and spin space. In the traditional *p*-wave superconductors the order parameter varies over the Fermi surface, and scattering of a Cooper pair from the states \mathbf{k} , $-\mathbf{k}$ into \mathbf{k}' , $-\mathbf{k}'$ results in their decoherence. Consequently, superconductivity dies when the elastic scattering rate becomes comparable to the order parameter, $1/\tau \rightarrow \Delta$. Our result shows that decoherence effects in the spin-triplet, orbital-singlet paired state are significantly suppressed, and superconductivity survives much stronger levels of disorder until $(m/\mu)^2/\tau \rightarrow \Delta$.

To show quantitatively the effect of disorder on the onset of superconductivity, we examine the pairing susceptibility near the transition. First, we transform into the eigenstate basis, in which the Hamiltonian is diagonal, $H_0 = \sum_{\mathbf{k},j} E(\mathbf{k}) [c_j^\dagger(\mathbf{k}) c_j(\mathbf{k}) - d_j^\dagger(\mathbf{k}) d_j(\mathbf{k})]$, where the dispersion is $E(\mathbf{k}) = \sqrt{m^2 + v^2(k_x^2 + k_y^2) + v_z^2 k_z^2}$. Despite the strong spin-orbital mixing in H_0 , the presence of both time-reversal and inversion symmetries protects the twofold degeneracy of the upper (c_1, c_2) and lower (d_1, d_2) bands at every \mathbf{k} . We chose to work in a particular basis [25], which we dub *pseudochiral*, where the states at \mathbf{k} and $-\mathbf{k}$ are related (up to a \mathbf{k} -dependent phase factor) by time-reversal (Θ) and inversion (P) operations:

$$\begin{aligned} \Theta c_1(\mathbf{k}) \Theta^{-1} &\sim c_1(-\mathbf{k}), & \Theta c_2(\mathbf{k}) \Theta^{-1} &\sim c_2(-\mathbf{k}), \\ P c_1(\mathbf{k}) P^{-1} &\sim c_2(-\mathbf{k}), & P c_2(\mathbf{k}) P^{-1} &\sim c_1(-\mathbf{k}). \end{aligned} \quad (3)$$

As long as the Hamiltonian has both time-reversal and inversion symmetries, it is always possible to use the basis satisfying the transformation properties described in Eq. (3).

In the pseudochiral basis, the superconducting order parameters (2a) and (2b) are given by:

$$\Delta_1(\mathbf{k}) \propto e^{-i\phi} \sum_{j=1,2} (-1)^j [\langle c_j(\mathbf{k}) c_j(-\mathbf{k}) \rangle + \langle d_j(\mathbf{k}) d_j(-\mathbf{k}) \rangle], \quad (4a)$$

$$\begin{aligned} \Delta_2(\mathbf{k}) \propto e^{-i\phi} \cos \alpha_{\mathbf{k}} \sum_{j=1,2} [\langle c_j(\mathbf{k}) c_j(-\mathbf{k}) \rangle - \langle d_j(\mathbf{k}) d_j(-\mathbf{k}) \rangle] \\ - 2e^{-i\phi} \sin \alpha_{\mathbf{k}} [\langle c_1(\mathbf{k}) d_2(-\mathbf{k}) \rangle + \langle c_2(\mathbf{k}) d_1(-\mathbf{k}) \rangle]. \end{aligned} \quad (4b)$$

In the derivation of the above expressions and from now on we rescaled the z component of the momentum by its velocities, $\mathbf{k} = (k_x, k_y, v_z k_z/v)$. While the expressions for the order parameters contain the azimuthal angle ϕ between (k_x, k_y) and the x axis, they are independent of the polar angle θ between \mathbf{k} and the z axis. The parameter $\alpha_{\mathbf{k}} = \sin^{-1}[m/E(\mathbf{k})]$ is a consequence of interorbital mixing by the mass term.

In the limit $m = 0$ ($\alpha_{\mathbf{k}} = 0$), the $\mathbf{k} \cdot \mathbf{p}$ Hamiltonian has a $U(1)$ chiral symmetry, $[H_0, \sigma_y s_z] = 0$. Thus, the energy eigenstates labeled by $j = 1(2)$ have a well-defined chirality $+1(-1)$, which is evident from Eq. (4). Importantly, pairing in both the even- and odd-parity states only occur between electrons of the same chirality, but the order parameters differ by the relative phase between Cooper pairs of opposite chirality (of different label j), π for Δ_1 and 0 for Δ_2 [7]. Since scalar disorder potential (which is insensitive to orbitals and spins) does not break chiral symmetry, impurities can scatter electrons only between states of equal chirality. Hence, the disorder affects the even-parity pairing Δ_1 and odd-parity pairing Δ_2 in the same way. Then, it follows from the Anderson theorem [20] that as long as the system is far from localization, both pairings are completely robust against disorder. The magnitudes of two order parameters at zero temperature differ only by the strength of the pairing interaction in the two channels, $\Delta_{\ell=1,2} = \Omega \exp\{-1/\nu_0 \lambda_\ell\}$ with ν_0 the density of states at the Fermi energy, λ_ℓ the attractive interaction in the even- or odd-parity channel, and Ω an ultraviolet cutoff.

For nonzero m in the Hamiltonian H_0 , the Bloch wave functions are no longer chiral eigenstates, and the similarity between the two order parameters is broken. Without loss of generality, we assume that the chemical potential lies in the upper energy band, $\mu > |m|$. Since only electrons on the Fermi surface contribute to the divergent pairing susceptibility at low temperature, the *effective* pairing order parameter involves only the c electrons of the conduction bands:

$$\Delta_1(\mathbf{k}) \propto e^{i\phi} [\langle c_1(\mathbf{k}) c_1(-\mathbf{k}) \rangle - \langle c_2(\mathbf{k}) c_2(-\mathbf{k}) \rangle], \quad (5a)$$

$$\Delta_2(\mathbf{k}) \propto e^{i\phi} \cos \alpha [\langle c_1(\mathbf{k}) c_1(-\mathbf{k}) \rangle + \langle c_2(\mathbf{k}) c_2(-\mathbf{k}) \rangle]. \quad (5b)$$

Here $\alpha = \sin^{-1}(m/\mu)$ is evaluated at the Fermi energy. One can see that for $m \neq 0$ the effective pairing potential in the odd-parity channel between electrons in the conduction bands is reduced due to mixing with the valence electrons [see Eq. (4b)]. Assuming the strength of the

interorbital attraction is independent of the parameter m/μ , the magnitude of the odd-pairing order parameter at zero temperature becomes $\Delta_2 = \Omega \exp\{-1/\nu_\alpha \cos^2 \alpha \lambda_\ell\}$. The order parameter Δ_2 is reduced from its $m = 0$ not only due to the dependence of the density of states on m/μ , $\nu_\alpha = \nu_0 \cos \alpha$, but mainly because the attractive interaction is weaker by a factor of $\cos \alpha$. We wish to emphasize that this change in the odd-symmetry order parameter is not caused by pair breaking. Pair breaking effects reduce the transition temperature, but not the zero temperature order parameter [26].

Introducing scattering by a scalar disorder potential adds a term into the Hamiltonian which is nondiagonal in the momentum, $H(\mathbf{k}, \mathbf{k}') = H_0(\mathbf{k})\delta_{\mathbf{k},\mathbf{k}'} + V_{\text{imp}}\psi^\dagger(\mathbf{k})\psi(\mathbf{k}')$. Transforming into the pseudochiral basis, one can see that the impurities mix all bands. However, in the limit $\varepsilon_F \tau \gg 1$, all leading order processes occur near the Fermi surface, and we can again restrict our attention to the conduction bands. The matrix element between two states at the Fermi energy, $\psi_i(\mathbf{k})$ and $\psi_j(\mathbf{k}')$, is given by

$$V_{\mathbf{k},\mathbf{k}'}^{i,j} = \begin{pmatrix} A(\mathbf{k}, \mathbf{k}') & A(\mathbf{k}, -\mathbf{k}') \sin \alpha \\ A(-\mathbf{k}, \mathbf{k}') \sin \alpha & A(-\mathbf{k}, -\mathbf{k}') \end{pmatrix}. \quad (6)$$

Here $A(\mathbf{k}, \mathbf{k}') = V_{\text{imp}}[e^{i(\phi-\phi')} \cos \frac{\theta}{2} \cos \frac{\theta'}{2} + \sin \frac{\theta}{2} \sin \frac{\theta'}{2}]$ is equal to the wave function overlap between two spins pointing along \mathbf{k} and \mathbf{k}' directions. In the limit $m = 0$ ($\alpha = 0$) the off-diagonal matrix elements vanish, restoring the chiral symmetry.

To find the corrections to the electron self-energy Σ due to scattering by disorder we use the self-consistent Born approximation. Then the self-energy matrix for the two conduction bands is diagonal and determined by two processes, intraband scattering and scattering between the two conduction bands [for illustration see Fig. 1(a)]. The self-energy is found from the following self-consistent equation:

$$\Sigma_{\mathbf{k},\omega_n} \equiv -\frac{i}{2\tau} \text{sgn}(\omega) = \int \frac{d\mathbf{k}'}{(2\pi)^3} |V_{\mathbf{k},\mathbf{k}'}^{i,i}|^2 G_{\mathbf{k}',\omega_n}^i + \int \frac{d\mathbf{k}'}{(2\pi)^3} V_{\mathbf{k},\mathbf{k}'}^{i,j\neq i} V_{\mathbf{k},\mathbf{k}'}^{j\neq i,i} G_{\mathbf{k}',\omega_n}^j, \quad (7)$$

where $G_i^{-1}(\mathbf{k}, \omega_n) = i\omega_n - [E(\mathbf{k}) - \mu] - \Sigma(\mathbf{k}, \omega_n)$ is the Matsubara Green's function of the electrons in the band i . Examining the above equation, one can see that the two scattering processes interfere constructively. Consequently, the elastic scattering time satisfies $1 = \pi\nu_\alpha V_{\text{imp}}^2 \tau (1 + \sin^2 \alpha)$.

As we explained above, while the transition temperature is highly sensitive to pair decoherence mechanisms, the zero temperature order parameter is not modified. Therefore, we calculate the transition temperature into the superconducting phase for the even- and odd-pairing states from the corresponding pairing susceptibilities of the normal state:

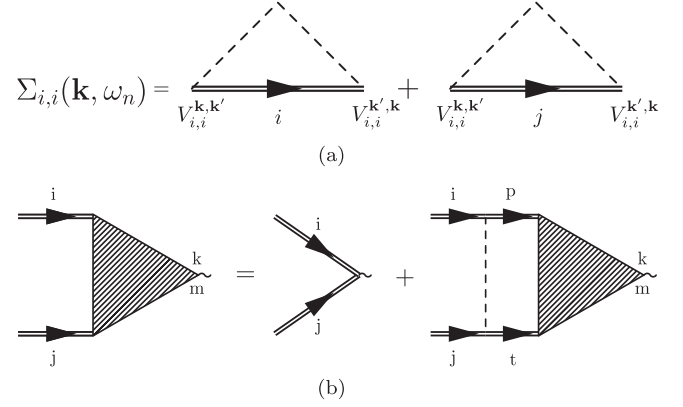


FIG. 1. The effect of disorder on the single particle Green's function and pair susceptibility. The self-consistent equation for the self-energy [Eq. (7)] is illustrated in (a). The double line represents the dressed electron Green's function, and the dashed line denotes the impurities. The equation for the Cooperon [Eq. (9)] is illustrated in (b). Here, the Cooperon is drawn as a filled triangle vertex.

$$\chi^\ell = \lambda T \sum_{i,j,k,m} \Gamma_{i,j}^\ell G_{\mathbf{k},\omega_n}^i G_{-\mathbf{k},-\omega_n}^j C_{i,j;k,m}(\omega_n) \Gamma_{k,m}^\ell. \quad (8)$$

Here, $\Gamma_{i,j}^\ell = \delta_{i,j}[\delta_{i,1} - \delta_{i,2}]$ for the spin-singlet pairing $\ell = 1$, and $\Gamma_{i,j}^\ell = \delta_{i,j} \cos \alpha [\delta_{i,1} + \delta_{i,2}]$ for the orbital-singlet pairing $\ell = 2$. The matrix $C_{i,j;k,m}(\omega_n)$ is the Cooperon describing multiple scattering events of two electrons (a Cooper pair) in the particle-particle channel. A pole in the Cooperon at $\omega_n = 0$ means that scattering by impurities does not result in decoherence of Cooper pairs. In other words, the probability of an electron in state \mathbf{k} to be scattered into state \mathbf{k}' is equal to the probability of its partner to be scattered into the partner of \mathbf{k}' . A Cooperon with a finite mass, on the other hand, implies that pairing is suppressed by disorder and that in the superconducting state there are subgap excitations.

The Cooperon can be expressed in terms of the single particle Green's function and impurity scattering potential:

$$C_{i,j;k,m}(\omega_n) = \delta_{i,k} \delta_{j,m} + \sum_{p,t=1,2} \int \frac{d\mathbf{k}'}{(2\pi)^3} \times V_{\mathbf{k},\mathbf{k}'}^{i,p} V_{-\mathbf{k},-\mathbf{k}'}^{j,t} G_{\mathbf{k}',\omega_n}^p G_{-\mathbf{k}',-\omega_n}^t C_{p,t;k,m}(\omega_n). \quad (9)$$

The only four components of the Cooperon that enter the susceptibilities are $C_{i,i;j,j}$. In the absence of impurities $C_{1,1;2,2} = C_{2,2;1,1} = 0$ and only the two components $C_{1,1;1,1} = C_{2,2;2,2}$ matter. As a result, there is no difference in the effect of disorder on both order parameters.

Similar to the single-particle self-energy, the Cooperon includes processes in which the electrons remain in the same band after scattering and those in which at least one

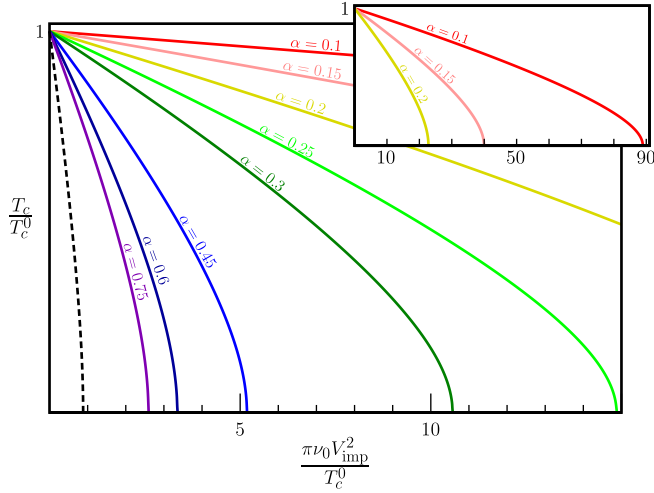


FIG. 2 (color online). The critical temperature as a function of the level of disorder $\pi\nu_0 V_{\text{imp}}^2$ for various values of α . Both T_c and $\pi\nu_0 V_{\text{imp}}^2$ are given in units of T_c^0 , the critical temperature for $V_{\text{imp}} = 0$. For comparison, the dashed line shows the transition temperature into the odd-parity superconducting state in the absence of spin-orbital locking (as in Helium-III). One can see that up to $\alpha \approx 0.5$ the critical level of disorder in which the unconventional order parameter disappears is dramatically higher than in Helium-III.

electron changes its band. However, while the interference between the scattering events that determine the elastic scattering time is constructive, the Cooperon is a sum of constructive and destructive interference terms. This can be seen in the expressions for $C_{i,i;j,j}$:

$$C_{i,i;j,j} = \frac{1 + 2|\omega_n|\tau}{1 + 2|\omega_n|\tau - \pi\nu_\alpha V_{\text{imp}}^2 \tau (1 - \sin^2\alpha)} + (-1)^{i+j} \frac{1 + 2|\omega_n|\tau}{1 + 2|\omega_n|\tau - \pi\nu_\alpha V_{\text{imp}}^2 \tau (1 + \sin^2\alpha)}. \quad (10)$$

Note that the above expression for the Cooperon has been calculated only assuming that $\varepsilon_F \tau \gg 1$. Now the two susceptibilities, χ^1 and χ^2 , are no longer identical. The even-pairing susceptibility includes only the constructive interference processes, $\chi^1 = 4\pi T \sum_{\omega_n} \nu_\alpha \tau [1 - \pi\nu_\alpha V_{\text{imp}}^2 \tau (1 + \sin^2\alpha)(1 - 2|\omega_n|\tau)]^{-1} = 2\pi T \sum_{\omega_n} \nu_\alpha / |\omega_n|$, and is clearly insensitive to disorder. In contrast, the susceptibility for odd-pairing is determined by the destructive interference, and hence, affected by impurities:

$$\chi^2 = T \sum_{\omega_n} \frac{\pi\nu_\alpha \cos^2\alpha}{|\omega_n| + \sin^2\alpha/\tau(1 + \sin^2\alpha)} = 2\nu_\alpha (\cos^2\alpha) \left[\ln \frac{\Omega}{2\pi T} - \psi \left(\frac{1}{2} + \frac{\sin^2\alpha}{2\pi T(1 + \sin^2\alpha)\tau} \right) \right], \quad (11)$$

where $\psi(x)$ is the digamma function.

Let us explain the above result. The pair decoherence rate, $1/\tau_\varphi = (\sin^2\alpha)/(1 + \sin^2\alpha)\tau$, which reduces the transition temperature enters the Cooperon as a mass term eliminating its divergence. When $1/\tau_\varphi$ is larger than the order parameter in the absence of pair decoherence, superconductivity disappears. We found that disorder introduces a pair breaking mechanism for the odd-parity pairing but not for the even-parity pairing, and that the key difference between the two-order parameters is the phase between the condensates in the two conducting bands. Therefore, we conclude that the decoherence is due to the tendency of the impurity scattering to favor a relative phase of π between the conduction bands (the singlet pairing), suppressing the spin-triplet transition temperature:

$$\ln \frac{T_c(\tau)}{T_c^0} = \psi \left(\frac{1}{2} \right) - \psi \left(\frac{1}{2} + \frac{1}{2\pi T_c(\tau)\tau_\varphi} \right). \quad (12)$$

Here we use T_c^0 to denote the transition temperature at $1/\tau = 0$ and finite α , and $C = \pi/2e^\gamma$ with γ the Euler constant. The suppression of T_c as a function of disorder for various values of α is illustrated in Fig. 2.

To understand better the peculiarity of this result, it is instructive to compare our result, applicable for the narrow-gap semiconductors, with the Ballian-Werthamer superfluid phase in He-III. Although the latter has a single band without spin-orbit coupling, one can choose a basis in which spin is locked to be parallel, $\phi_1(\mathbf{k})$, or antiparallel, $\phi_2(\mathbf{k})$ to the momentum. This basis ϕ resembles the chiral basis we used here. Correspondingly, in both cases the odd-parity order parameters can be written as $e^{i\phi}[\phi_1(\mathbf{k})\phi_1(-\mathbf{k}) + \phi_2(\mathbf{k})\phi_2(-\mathbf{k})]$. The key difference between systems with and without spin-orbital locking manifests itself in the impurity scattering. While in helium-III, the matrix element for impurity scattering between $\phi_1(\mathbf{k})$ and $\phi_2(\mathbf{k}')$ are larger than the diagonal terms, in the problem studied here the interband scattering is parametrically smaller than the intraband one by a factor of $\sin\alpha = m/\mu$, due to the approximate chiral symmetry that becomes exact as $m \rightarrow 0$. Thus, the pair decoherence in the narrow-gap semiconductors is significantly weaker than in Helium-III. Note that this observation is only correct for scalar disorder, and does not hold for other types of scattering potentials, such as magnetic impurities ($\propto \vec{s}$) or orbital dependent potentials ($\propto \vec{\sigma}$). These non-scalar disorder potentials cause stronger pair decoherence and suppress the unconventional superconducting state.

Our result can be generalized to 2D bilayer band structures obtained by setting $k_z = 0$ in the $k \cdot p$ Hamiltonian (1). Recently, it has been proposed [27] that this class of bilayer systems with Rashba spin-orbit coupling favors odd-parity superconductivity similar to the 3D case. Our analysis shows a similar robustness against disorder due to the chiral symmetry (See Supplemental Material [28]).

To conclude, we showed that certain types of odd-parity pairing in doped narrow-gap semiconductors can survive from a fairly large amount of impurity scattering. The relative robustness of these systems results from an approximate chiral symmetry in the spin-orbital locked band structure *and* the odd-parity pairing order parameter. Although scattering by disorder reduces the phase coherence of the Cooper pairs, the dephasing rate $1/\tau_\phi = \pi\nu_\alpha V_{\text{imp}}^2 \sin^2\alpha$ vanishes as the Dirac mass (= band gap) in the band structure goes to zero, when the chiral symmetry becomes exact. Finally, we note that in addition to centrosymmetric materials studied in this work, strong spin-orbit-coupling in asymmetric interface structures can also protect unconventional superconductivity against disorder [29].

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