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Unconventional pairings and radial line nodes in inversion symmetry broken superconductors

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ABSTRACT

Noncentrosymmetric superconductors (NCSs) with broken inversion symmetry can have spin-dependent order parameters (OPs) with mixed parity which can also have nodes in the pair potential as well as the energy spectra. These nodes are distinct features that are not present in conventional superconductors. They appear as points or lines in the momentum space where the latter can have angular or radial geometries dictated by the dimensionality, the lattice structure and the pairing interaction.

In this work we study the nodes in time reversal symmetry (TRS) preserving NCSs at the OP, the pair potential, and the energy spectrum levels. Nodes are examined by using spin independent pairing interactions respecting the rotational $C_{\infty v}$ symmetry in the presence of spin-orbit coupling (SOC). The pairing symmetries and the nodal topology are affected by the relative strength of the pairing channels which is studied for the mixed singlet-triplet, pure singlet, and pure triplet. Complementary to the angular line nodes widely present in the literature, the $C_{\infty v}$ symmetry here allows radial line nodes (RLNs) due to the nonlinear momentum dependence in the OPs. The topology of the RLNs in the mixed case shows a distinctly different characterization than the half-spin quantum vortex at the Dirac point. We apply this NCS physics to the inversion symmetry broken exciton condensates (ECs) in double quantum wells where the point and the RLNs can be found. On the other hand, for a pure triplet condensate, two fully gapped and topologically distinct regimes exist, separated by a QSHI-like zero energy superconducting state with even number of Majorana modes. We also remark on how the point and the RLNs can be manipulated, enabling an external control on the topology.

Pairing symmetries beyond the conventional BCS have been first addressed in the B and the A phases of ^3He [1,2]. Unconventional pairing states were then reported in heavy fermion [3] and the high-T_c superconductors [4]. It is now settled that, the inversion symmetry (IS), the time reversal , the particle-hole (Λ) and the fermion exchange (F_X) i.e. Pauli exclusion symmetries play fundamental role in unconventional superconducting pairing.

In the NCSs the IS is broken. They comprise a subset of a larger class, i.e. unconventional superconductors. The broken IS is usually connected to the presence of a SOC which requires mixed parity OPs, i.e. the even parity singlet (s) is mixed with the odd parity triplet (t). The broken IS does not mean a strong triplet, but a weakly broken IS means a singlet dominant mixed state. For instance, NMR measurements yield that Li_2Pt_3B is a mixed s-t state with a strong SOC [5] whereas Li_2Pd_3B is believed to be s-dominated with a weak SOC [6]. On the other hand, $BaPtSi_3$ [7] as well as *SrPtAs* [8] are known to break IS but they were reported as BCS like pure singlets. Usually, it is experimentally hard to separately identify a dominating singlet (triplet) within a mixed state from a pure singlet (triplet).

A comprehensive understanding of the pairing mechanisms in NCS is currently far from complete [9]. The IS breaking is fundamentally important for spin dependent mixed parity OPs, but it needs to be sufficiently large for the nodes to appear. In TRS manifested NCSs nodes appear either at the time-reversal-invariant points or lines at certain angular orientations dictated by the crystal symmetry. Another crucial point is that, nodes in the OPs do not necessarily mean nodes in the pair potential or the energy spectrum. In centrosymmetric materials with tetragonal symmetry, strong Hubbard-like electronic correlations or spin fluctuations around AFM nesting can lead to the natural separation of the s and t pairing channels without an explicit need of an IS breaking [10]. On the other hand, phonon mechanisms were suggested for some

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NCSs [11]. Independently from the details of the mechanism, it is crucial that the interaction symmetries should allow the simultaneous presence of a sufficiently large triplet with or without a singlet. The triplet/singlet ratio as a function of momentum is therefore an important parameter in understanding the nodes. Nodes are also closely connected with the topology of the momentum space. All these factors outlined here point at the need for more simplistic approaches stressing the self-consistent handling of interactions with realistic momentum dependence as the key for a broader understanding of the physics of NCSs.

In this work we focus on four questions that can help our understanding: a) In NCSs, can we identify factors affecting the unconventional pairings without resorting to any lattice or other material dependent symmetries and interactions?, b) How does a pairing interaction affect the nodal structure of the OPs, the pair potential and the spectrum? c) Can the nodes, and hence the topology, be controlled externally? d) How does the nodal topology in the pair potential or spectrum in an NCS relate to a topological superconductor (TSC)?

To answer these questions we use a material independent model with maximal rotational symmetry. We also confine our attention to two dimensions. The model consists of an IS breaking SOC and an isotropic, *spin independent* pairing interaction $\mathcal{V}(q)$ with repulsive and attractive parts. This *minimal model* has $C_{\infty v}$ as the simplest rotational symmetry with no referral to any specific discrete point group. Our conclusions are therefore expected to be applicable to the material independent and general aspects of pairing in TRS manifested NCSs such as those under weak anisotropy. With these inputs, we examine the relation between the pairing interaction, the pairing symmetries and the nodes.

The two dimensional mean field Hamiltonian we consider is described in the electronic basis $\Psi_{\mathbf{k}}^\dagger = (\hat{e}_{\mathbf{k}\uparrow}^\dagger\ \hat{e}_{\mathbf{k}\downarrow}^\dagger\ \hat{e}_{-\mathbf{k}\uparrow}\ \hat{e}_{-\mathbf{k}\downarrow})$ where Nambu and the spin sectors are denoted respectively by the Pauli matrices $\tau = \{\tau_x, \tau_y, \tau_z\}$ and $\sigma = \{\sigma_x, \sigma_y, \sigma_z\}$. The Hamiltonian is [12]

$$\mathcal{H} = \sum_{\mathbf{k}} \Psi_{\mathbf{k}}^\dagger \mathcal{H}_{\mathbf{k}} \Psi_{\mathbf{k}}, \quad \mathcal{H}_{\mathbf{k}} = \mathcal{H}_{\mathbf{k}}^0 + \mathcal{H}_{\mathbf{k}}^{soc} + \mathcal{H}_{\mathbf{k}}^{\Delta}. \tag{1}$$

Here, $\mathcal{H}_{\mathbf{k}}^0 = \tau_z \otimes \widehat{\xi}_k$ where $\widehat{\xi}_k = [\hbar^2 k^2/(2m) - \mu]\sigma_0 + \widehat{\Sigma}_k$, m is the band mass, μ is the Fermi energy, $\widehat{\Sigma}_k$ is the 2 × 2 self energy matrix in the spinor basis, $\mathcal{H}_{\mathbf{k}}^{soc} = [(S_{\mathbf{k}} \hat{e}_{\mathbf{k}\uparrow}^\dagger \hat{e}_{\mathbf{k}\downarrow} + S_{\mathbf{k}}^* \hat{e}_{-\mathbf{k}\uparrow} \hat{e}_{-\mathbf{k}\downarrow}^\dagger) + h.c]$ is the SOC Hamiltonian and $S_{\mathbf{k}} = \alpha\, k\, exp(i\phi_{\mathbf{k}})$ is the SOC. Here $k = |k_x + ik_y|$ is the inplane wavevector, $\alpha = \gamma_0 E_z$ with γ_0 is a material dependent constant [13,14], E_z is an external electric field and $exp(i\phi_{\mathbf{k}}) = (k_x + ik_y)/k$ is the SOC phase. The third term in Eq. (1) is the pairing Hamiltonian $\mathcal{H}_{\mathbf{k}}^{\Delta} = \tau_+ \otimes \widehat{\Delta}_k + h.c.$ where $\tau_\pm = \tau_x \pm i\tau_y$ and $\widehat{\Delta}_k = i[\psi_{\mathbf{k}}\sigma_0 + \mathbf{d}_{\mathbf{k}}.\sigma]\sigma_y$ is the spin dependent mixed OP with $\psi_{\mathbf{k}}$ and $\mathbf{d}_{\mathbf{k}} = \{d_{x\mathbf{k}}, d_{y\mathbf{k}}, d_{z\mathbf{k}}\}$ as the even singlet ($\psi_{\mathbf{k}} = \psi_{-\mathbf{k}} = \psi_k$) and the odd triplet ($\mathbf{d}_{\mathbf{k}} = -\mathbf{d}_{-\mathbf{k}}$) respectively. [1,9] The mixed OP can also be written as

$$\widehat{\Delta}_k = \begin{pmatrix} \Delta_{\uparrow\uparrow}(\mathbf{k}) & \Delta_{\uparrow\downarrow}(\mathbf{k}) \\ \Delta_{\downarrow\uparrow}(\mathbf{k}) & \Delta_{\downarrow\downarrow}(\mathbf{k}) \end{pmatrix} \tag{2}$$

In the triplet, $d_{x\mathbf{k}} = (\Delta_{\downarrow\downarrow} - \Delta_{\uparrow\uparrow})/2$, $d_{y\mathbf{k}} = (\Delta_{\downarrow\downarrow} + \Delta_{\uparrow\uparrow})/(2i)$ are the equal-spin pairings (ESP), $d_{z\mathbf{k}} = (\Delta_{\uparrow\downarrow} + \Delta_{\downarrow\uparrow})/2$ is the opposite-spin-paired (OSP) triplet, whereas $\psi_k = (\Delta_{\uparrow\downarrow} - \Delta_{\downarrow\uparrow})/2$ is the singlet. Denoting the time reversal transformation by Θ, TRS is manifested when $\Delta_{\sigma\sigma'}(\mathbf{k}) = \Theta : \Delta_{\sigma\sigma'}(\mathbf{k}) = \lambda_\sigma \lambda_{\sigma'} \Delta_{\bar{\sigma}\bar{\sigma}'}^*(-\mathbf{k})$ where $\lambda_\uparrow = 1$, $\lambda_\downarrow = -1$ and $\bar{\sigma}$ is anti-parallel to σ. When F_X and TRS are simultaneously manifested, the OPs satisfy a strong condition $\Delta_{\sigma\bar{\sigma}}(\mathbf{k}) = \Delta_{\sigma\bar{\sigma}}^*(\mathbf{k})$ implying that ψ_k and $d_{z\mathbf{k}}$ are real. Additionally, the $C_{\infty v}$ symmetry requires that the order parameters are functions of k only. These conditions together imply that $\psi_k d_{z\mathbf{k}} \propto (|\Delta_{\uparrow\downarrow}|^2 - |\Delta_{\downarrow\uparrow}|^2) = 0$. Hence the simultaneous admixture of the singlet and the OSP triplet should be suppressed in the TRS manifested and weakly anisotropic NCSs [15].

Table 1
Possible configurations allowed in the minimal model with $C_{\infty v}$ symmetry for the s-t pairing. Here $\sigma = (\uparrow, \downarrow)$ and we consider manifested/broken TRS and IS. Here ψ_k, F_k and D_k are radial functions of k. Note that the cases i-vi are allowed in the minimal model irrespective of the isotropic and spin-independent pairing interaction $V(q)$.

Case	TRS	IS	$\Delta_{\sigma\sigma}(\mathbf{k})$ (ESP)	$d_{z\mathbf{k}}$ (OSP)	ψ_k (OSP)
i	✓	✓	0	0	ψ_k (real)
ii	✓	×	$\lambda_\sigma F_k e^{i\lambda_\sigma \phi_{\mathbf{k}}}$	0	ψ_k (real)
iii	✓	×	0	0	ψ_k (real)
iv	✓	×	$\lambda_\sigma F_k e^{i\lambda_\sigma \phi_{\mathbf{k}}}$	0	0
v	×	×	0	$D_k e^{\pm i\phi_{\mathbf{k}}}$	0
vi	×	×	$\lambda_\sigma F_k e^{i\lambda_\sigma \phi_{\mathbf{k}}} e^{i\theta_k^{(t)}}$	0	$\psi_k e^{i\theta_k^{(s)}}$

Under these conditions all relevant pairings allowed in the ground state of $\mathcal{H}$ in Eq. (1) are listed in Table 1 as i) a mixed singlet-ESP triplet (s-t_{ESP}) in TRS and spontaneously broken TRS (SBTRS) phases, ii) a pure s in TRS phase, and iii) two pure triplet (t_{ESP}) and (t_{OSP}) respectively in TRS and SBTRS phases.

In the TRS phase, the triplet is dictated by unitarity to have the form $\mathbf{d}_{\mathbf{k}} = (-F_k \cos\phi_{\mathbf{k}}, F_k \sin\phi_{\mathbf{k}}, 0)$ where F_k is the ESP strength. In NCSs, the TRS preserving m-state is experimentally the most common ground state, with Li_2Pt_3B [5], $CePt_3Si$ [16] and $CaTSi_3$ (T:Ir,Pt) [17] as few examples. As far as the phases in the minimal model are concerned, the m-state as energetically the most stable configuration in almost all parameter ranges of the pairing interactions used, unless one of the angular momentum channels is specifically turned off. The TRS preserving pure t_{ESP} is similar to the ^3He-B phase (BW state). In the SBTRS phase a t_{OSP} is found similar to the ^3He-A phase (ABM state, case v). The other SBTRS solution is a mixed state like in $LaNiC_2$ [18] (case vi). Hence, the minimal model alone, characterized by the $C_{\infty v}$ symmetry, is capable of producing a number of common pairing symmetries respecting or violating the TRS as shown in Table 1. In this work, we will confine ourselves only to the TRS regime described by the cases i–iv in the Table 1.

The mean field calculations yield that the s-t OPs are coupled in the minimal model by,

$$\psi_k = -\frac{1}{A}\sum_{k',\lambda} \mathcal{V}_s(k,k') \frac{\tilde{\Delta}_{k'}^{\lambda}}{4E_{k'}^{\lambda}} \left\{ f(E_{k'}^{\lambda}) - f(-E_{k'}^{\lambda}) \right\}$$
$$F_k = \frac{1}{A}\sum_{k',\lambda} \mathcal{V}_t(k,k') \frac{\lambda\tilde{\Delta}_{k'}^{\lambda}}{4E_{k'}^{\lambda}} \left\{ f(E_{k'}^{\lambda}) - f(-E_{k'}^{\lambda}) \right\} \tag{3}$$

where $\tilde{\Delta}_k^{\lambda} = (\psi_k - \lambda\gamma_k F_k)$ with the $\lambda = \pm$ signs refer to the SOC dependent splitting, $\gamma_k = sgn(|G_{\mathbf{k}}|\xi_k - F_k\psi_k)$ with $G_{\mathbf{k}} = S_{\mathbf{k}} + (\Sigma_k)_{\uparrow\downarrow}$. Here $(\Sigma_k)_{\uparrow\downarrow}$ is the nondiagonal element of the self-energy matrix as given similarly to Eq. (2) and $f(x) = 1/[exp(\beta x) + 1]$ is the Fermi-Dirac factor. The eigen energies are

$$E_k^{\lambda} = \sqrt{(\tilde{\xi}_k^{\lambda})^2 + (\tilde{\Delta}_k^{\lambda})^2} \tag{4}$$

where $\tilde{\xi}_k^{\lambda} = \xi_k + \lambda\gamma_k|G_{\mathbf{k}}|$. In NCS, the presence of SOC naturally separates the s and t pairing channels as V_s and V_t in Eq. (3), and a spin-dependent interaction, like Hubbard's U is not essentially needed for the s-t channel separation [19]. The pairing interaction $V(q)$ is isotropic and spin independent with the angular momentum expansion $V(q) = \sum_{n=-\infty}^{\infty} \tilde{\mathcal{V}}_n(k,k') e^{in\phi_{\mathbf{k}\mathbf{k}'}}$ where $\mathbf{q} = \mathbf{k} - \mathbf{k}'$, $\phi_{\mathbf{k}\mathbf{k}'} = (\phi_{\mathbf{k}} - \phi_{\mathbf{k}'})$ and n is the angular momentum quantum number. The s-t channel separation in Eq. (3) is specifically given