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Nodal line topological superconducting state in quasi-one-dimensional $A_2Cr_3As_3$ ($A = K, Rb, Cs$) superconductors

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In recent years, chromium-based superconductors such as $A_2Cr_3As_3$ ($A = K$, Rb, Cs) have attracted significant attention due to their unique properties and potential applications [1–3]. These materials are composed of well-separated $[(Cr_3As_3)^{2-}]_\infty$ chains and exhibit strong one-dimensional Tomonaga–Luttinger liquid behavior in the normal state [4–7].

In the superconducting state, these materials display unconventional superconducting characteristics. The unique properties of both normal and superconducting states in these materials have spurred considerable research interest in the $A_2Cr_3As_3$ system [8–12]. Pairing symmetry is a crucial aspect when investigating superconducting systems. For $A_2Cr_3As_3$ superconductors, some groups have theoretically predicted possible s-wave pairing [9, 13]. However, the high upper critical field that sharply increases to 44.7 T at 0 K, nearly four times the Pauli limit [14], provides stronger theoretical support for p-wave pairing symmetry, which exhibits potential topological characteristics [15, 16].

Moreover, the energy bands of p-wave $A_2Cr_3As_3$ superconductors bear similarities to three-dimensional topological nodal line semi-metals, which feature one-dimensional rings at the Fermi energy [17–21]. Theoretical predictions and experimental findings point to fascinating topological p-wave pairing and surface flat bands with a high density of states, motivating further investigations of superconductivity in the $A_2Cr_3As_3$ system.

In this paper, we explore the superconducting mechanisms and potential topological properties of chromium-based superconductors from a theoretical standpoint. We have developed a three-orbital tight-binding model in momentum space to qualitatively describe the superconducting performance of $A_2Cr_3As_3$ superconductors.

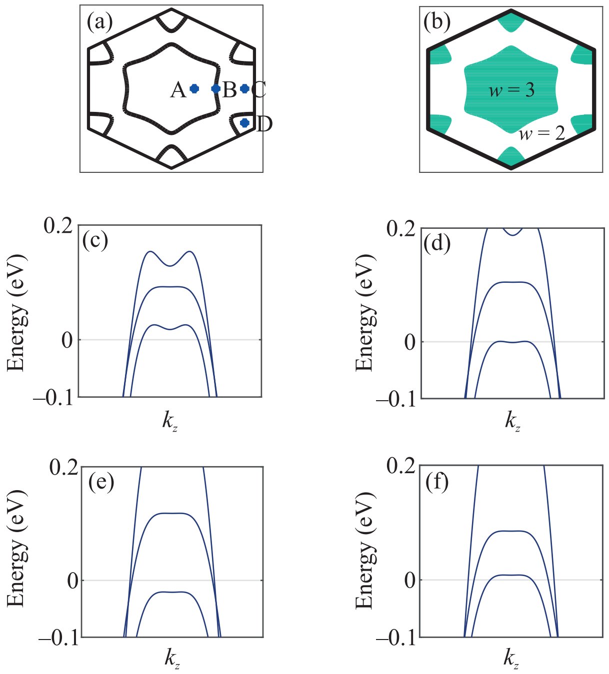

Fig. 1. (Color online) (a) – The normal state Fermi surface at the $k_z = 0$ plane. (b) – Phase diagram on the (k_x,k_y) plane. w is winding number. Panels (c)–(f) are the normal state energy bands as a function of k_z at the points A, B, C and D, respectively

As reported in [6, 11, 15], the normal Fermi surface is a three-dimensional pocket symmetrical about $k_z = 0$ plane. To study the system's topological properties, we must identify the critical points of different phases. For the p_z-wave pairing symmetry, the superconducting gap equals zero at the $k_z = 0$ plane. We plot the normal state Fermi surface on the $k_z = 0$ plane in Fig. 1a. It reveals

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1)e-mail: wliming@scnu.edu.cn; tzhou@scnu.edu.cn that the system is gapless in the normal state. It should also be the nodal line in the p_z-superconducting state.

Therefore, we introduce a chiral-protected momentum-dependent integral z-value topological invariant: winding number (w) and apply it to the $A_2Cr_3As_3$ family of materials [22–24]. The phase diagram is shown in Fig. 1b. Our results reveal that $A_2Cr_3As_3$ possesses non-trivial topology on the (k_x, k_y) plane. The phase diagram can be well understood by analyzing the normal state energy bands. Previously, the one-dimensional p-wave superconductor, specifically the one-dimensional Kitaev chain model, has been extensively studied [25]. The topological nature is determined by the normal state Fermi energy. We present the normal state energy bands for different points of the phase diagram in Figs. 1c–f. Then, in the p-wave superconducting state, all of these three bands contribute to the nontrivial topological superconductiveity, result in the $w = 3$ at this region. Two bands cross the Fermi energy, so that at this region, the topological invariant w reduces to 2. Non-zero topological invariants within the Fermi surface typically result in the presence of topologically protected zero-energy flat bands on the system surface. Our numerical calculations show that the entire Brillouin zone is covered by a completely flat energy band.

In order to further verify the topological properties of the system, we consider open boundary conditions along the x- and y-directions, and periodic boundary conditions along the z-direction. We plot the energy band, spectral function and zero energy spectrum function, which serve as valuable indicators of the system's topological properties. These numerical results confirm that the Brillouin zone's non-zero value results in precisely flat surface bands. And edge states and zero modes can be stabilized.

Notably, our work not only considers p-wave symmetry but also numerically verifies the absence of edge states in the superconducting state for s-wave pairing symmetry. Furthermore, we find that the system is topologically trivial for s-wave pairwise symmetry in the superconducting state.

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