

Fermi surface and topology of the multiband superconductor BeAu

Riccardo Vocaturo¹, Klaus Koepernik¹, Dániel Varjas^{1,2,3}, Oleg Janson¹,

Maia G. Vergniory^{4,5,6} and Jeroen van den Brink^{1,2,7}

¹*Leibniz Institute for Solid State and Materials Research (IFW) Dresden, Helmholtzstrasse 20, 01069 Dresden, Germany*

²*Würzburg-Dresden Cluster of Excellence ct.qmat, Helmholtzstrasse 20, 01069 Dresden, Germany*

³*Department of Theoretical Physics, Institute of Physics, Budapest University of Technology and Economics, Műegyetem rkp. 3., 1111 Budapest, Hungary*

⁴*Regroupement Québécois sur les Matériaux de Pointe (RQMP), H3T 3J7 Québec, Canada*

⁵*Donostia International Physics Center, 20018 Donostia-San Sebastian, Spain*

⁶*Département de Physique et Institut Quantique, Université de Sherbrooke, Sherbrooke, J1K 2R1 Québec, Canada*

⁷*Institute of Theoretical Physics, Technische Universität Dresden, 01062 Dresden, Germany*



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The chiral material BeAu was recently identified as a multiband type-I superconductor with a critical temperature of 3.2 K. As a member of the B20 crystal family (space group $P2_13$), its band structure hosts multifold fermions at high-symmetry points, unpaired WPs, and even nodal surfaces. This renders BeAu an appealing system for investigating the interplay between superconductivity and topology. Here, we present a comprehensive first-principles analysis of BeAu's electronic structure, focusing on its Fermi surface's topology and the implications for superconductivity. Together with the presence of four- and sixfold fermions at high-symmetry points, we identify several additional isolated WPs near the Fermi level. We also determine the associated topological edge states—the surface Fermi arcs. Computing the Chern number associated to different Fermi surface sheets, we show that BeAu harbors a $\nu = 4$ topological superconducting phase in the presence of s -wave pairing of alternating sign ($s_{\pm}$ pairing). Notably, we also identify a Fermi surface with a Chern number of $+6$; the highest value reported to date. Finally, our analysis reveals strong inhomogeneity in the orbital character of electronic states at the Fermi level, suggesting a link to the observed multigap superconductivity.

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I. INTRODUCTION

The family of B20 compounds has been gaining significant attention in recent years, presenting itself as a natural platform for investigating exotic topological phases [1]. Materials belonging to this family crystallize in the FeSi-type lattice, with chiral space group $P2_13$ (No. 198). This structure is characterized by the absence of inversion and mirror symmetries, and the presence of three screw-rotation axes along the unit cell's main diagonals. Such an uncommon combination of crystalline symmetries provides ideal conditions for realizing unconventional electronic features in the band structure. For instance, symmetry-enforced multiband crossings occur at high-symmetry points in the Brillouin zone (BZ), carrying topological charges as large as five [2]. These crossings, termed multifold fermions [3,4], have been extensively studied in recent years due to the possibility of yielding extremely long surface Fermi arcs [5], second-harmonic generation [6,7], quantized circular photogalvanic effect [8], and many more (nonlinear) transport properties [9–12].

Yet, multifold fermions are not the only unconventional features in chiral crystals. For example, space group 198 is among the few known cases where nodal surfaces (NS) and isolated Weyl points (WPs) can be found. Here, these two elements appear together and make it possible to circumvent the famous Nielsen–Ninomiya theorem, allowing the existence of a single WP in a periodic lattice. These types of excitations were first proposed in 2019 [13,14] and experimentally observed two years later in another B20 compound, PtGa [15].

Another aspect of great interest lies in the appealing prospect of realizing topological superconductivity. Qi *et al.* [16] showed that time-reversal-invariant Weyl semimetals can undergo a topological superconducting transition if the pairing function changes sign between Fermi surfaces (FSs) of different chirality. In the weak-coupling limit, the topological invariant is given by

$$\nu = \frac{1}{2} \sum_{i \in \text{FS}} C_i \text{sgn}(\Delta_i), \quad (1)$$

where Δ_i is the superconducting gap on the i -th FS, and C_i is its Chern number, computed as the flux of Berry curvature through the i -th sheet. In a conventional Weyl semimetal, $C_i = \pm 1$ for Fermi surfaces enclosing a WP and zero otherwise. While a sign-changing order parameter is not typically expected in conventional electron-phonon superconductors,

Hosur *et al.* [17] showed that second-order effects from Coulomb repulsion between different FSs can stabilize such a state, even in the presence of purely local interactions. In this context, B20 compounds are interesting because they host multifold fermions at high-symmetry points, giving rise to extended and well-separated Fermi surfaces with large Chern numbers. On the contrary, in conventional Weyl semimetals, WPs are usually located close to one another, resulting in a smaller probability of observing a sign change of the superconducting gap across the corresponding pockets. Significant attention has thus been devoted to the effect of superconductivity on the multifold fermions at the Γ and R points [18–20]. In minimal toy models, it has been predicted that $s_{\pm}$ pairing may even drive a topological superconducting transition with invariant $\nu = 4$ [21].

In this work, we turn our attention to BeAu, which, remarkably, exhibits a superconducting transition $T_c \approx 3.2$ K [22–24], despite the poor superconducting properties of both beryllium and gold. It is also one of only two known superconductors in the B20 family (the other being RhGe [25]). Additionally, multiple experimental evidence points toward the presence of multiband superconductivity in this system [26–28].

The agreement between the experimentally observed T_c and theoretical calculations [29] suggests that superconductivity in BeAu is primarily driven by electron-phonon coupling from light Be atoms; a mechanism reminiscent of high-pressure hydrides. However, the presence of two distinct superconducting gaps leaves two important questions unanswered: which FSs are involved, and what mechanism gives rise to their different gap magnitudes? Experimental data further hints that one of the gaps is strongly coupled while the other is weakly coupled [29], pointing toward a significant anisotropy in the interaction strength. This raises the possibility that an $s_{\pm}$ pairing may emerge despite the dominance of electron-phonon coupling, leading to a topological superconducting phase.

Since previous theoretical studies [21] were conducted at the effective model level, inevitably neglecting material-specific aspects, we present here a comprehensive first-principles investigation of the electronic structure of BeAu, with a particular focus on its Fermi surface. After a general overview of the crystal (Sec. II) and electronic (Sec. III) structure, we highlight the presence of known multifold fermions at the high-symmetry points (Sec. III A) and perform a systematic search throughout the BZ to identify WPs at generic positions, finding multiple *isolated* crossings in the proximity of the Fermi level (Sec. III B). We also examine in depth the surface spectral properties, discussing important aspects. In Secs. IV and V, we focus on the complex Fermi surface of this system, revealing additional electron and hole pockets beyond those at Γ and R points captured by the effective model in Ref. [21]. Moreover, the presence of several isolated crossings in the proximity of the Fermi level complicates the determination of the topological charge of each sheet, which is not easily inferred from a counting argument alone. Consequently, to rigorously confirm the possibility of a nontrivial topological invariant in the presence of $s_{\pm}$ superconductivity, we carry out a careful numerical computation of Fermi-surface Chern numbers.

Our main result is a complete topological characterization of the Fermi surface of BeAu, showing that it is consistent with the $\nu = 4$ topological superconducting phase theoretically proposed in minimal models [20,21]. We also identify a Fermi surface sheet with a Chern number of $C = 6$ which could, in principle, support even richer superconducting phases. To the best of our knowledge, this is also the highest value reported for a single Fermi surface. Finally, we find a highly anisotropic distribution of atomic orbital character at the Fermi level, a factor that could influence the electron-phonon interaction and help explain the origin of the observed multigap behavior.

II. CRYSTAL STRUCTURE

The low-temperature phase of BeAu emerges below 860 K [24], crystallizing in the chiral FeSi-type structure with the cubic unit cell parameter $a = 4.6699(4)$ Å at room temperature [22]. This structure type features sevenfold coordination polyhedra and represents an approximation to icosahedral quasicrystals [30].

The crystal structure belongs to the well-known space group $P2_13$ (No. 198), which is chiral due to the absence of both inversion symmetry and mirror planes. Its symmetry operations include a C_3 rotational axis along the $[111]$ direction and three nonsymmorphic screw rotations: $\{2_1(100) | \frac{1}{2} \frac{1}{2} 0\}$, $\{2_1(010) | 0 \frac{1}{2} \frac{1}{2}\}$, and $\{2_1(001) | \frac{1}{2} 0 \frac{1}{2}\}$. In this work, we will refer to such screw rotations with the notation $\tilde{C}_i$ with $i = x, y, z$. As structural input for our calculations, we use the experimental room-temperature structure where Au and Be occupy the $4a$ Wyckoff positions with coordinates $x_{\text{Au}} = 0.8549$ and $x_{\text{Be}} = 0.15$ [22].

III. ELECTRONIC STRUCTURE

To study the electronic structure of BeAu, we performed full-relativistic density functional theory (DFT) calculations using the full-potential local-orbital code FPLO [31] version 22.01-63. For the exchange-correlation term, we employed the generalized gradient approximation (GGA) [32]. The BZ was sampled by a $12 \times 12 \times 12$ mesh of k points. For slab calculations, a suitable Wannier representation was obtained through the dedicated FPLO module [33]. To do so, Kohn-Sham eigenstates were projected onto a basis of 80 spinfull orbitals that comprise Be $2s, 2p$ and Au $6s, 5d$; in an energy window between -9 and 5 eV. Our Wannier Hamiltonian is uploaded in Ref. [34]. For surface state calculations, we used the pyFPLO subroutine, which relies on the iterative algorithm presented in Ref. [35].

The band structure with and without spin-orbit coupling (SOC) is shown in Fig. 1(a), while in Fig. 1(b), we resolve atomic contributions of each band at each momentum. The density of states (DOS) has been previously published in Ref. [22,29]. In particular, it was shown that the Be and Au atomic contributions are essentially equal around E_F . This is consistent with Fig. 1(b), indicating strong hybridization of valence electrons in this compound. However, the atomic-resolved band structure evidences a quantitative difference in the orbital character of some states. For instance, the hole pocket around the M point has a remarkably higher Be

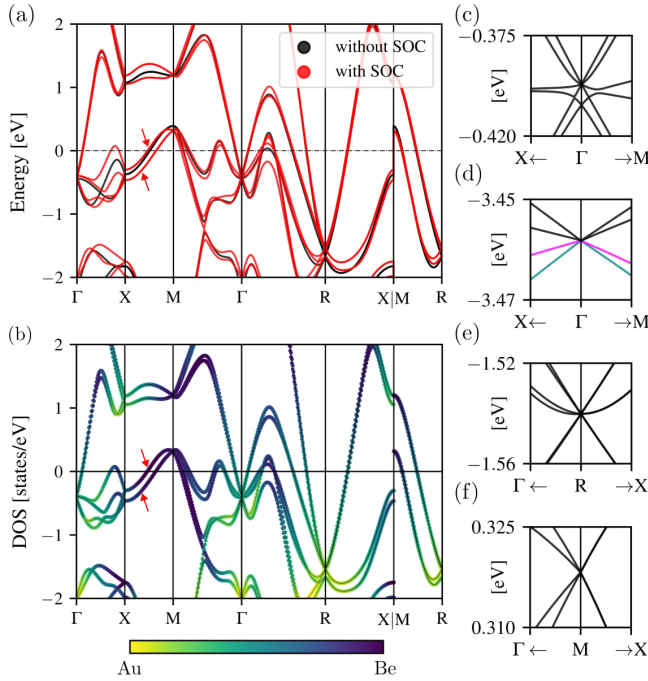


FIG. 1. (a) Scalar- (without SOC) and full-relativistic (with SOC) GGA band structures of BeAu. (b) Atomic-resolved full-relativistic band structure, highlighting the relative Au and Be contributions. (c)–(f) Zoom in on the multifold band crossing at high-symmetry points carrying nontrivial Chern numbers (full-relativistic band structure). In (d), we color in pink the band carrying $C = 5$ (see discussion in the main text for details).

contribution with respect to the neighboring bands crossing the Fermi level.

The impact of SOC can also be understood by comparing Fig. 1(a) to the orbital-resolved band structure in panel (b). As expected, Be, being a light element, induces negligible effects, while much wider band splitting is associated with regions of the BZ with stronger Au contribution. For instance, comparing Γ -M and M-X paths, we observe that along Γ -M, where the Be character dominates, the SOC-induced splitting is smaller. As we move toward Γ along the Γ -X direction, the splitting increases, in line with a higher Au contribution. In Ref. [36], the weaker spin-orbit splitting of Be-dominated states was invoked to explain the lower spin-Hall conductivity of this material compared to the Weyl semimetal TaAs or the conventional metal Pt. However, the same study also identified a significant amount of spin Berry curvature near the Fermi level, which results in a much higher spin-Hall conductivity relative to other B20 compounds.

Deriving an effective Hamiltonian describing the SOC for a generic 3D crystal is quite challenging, especially given the high number of bands present here. Alternatively, to provide an estimate of the characteristic strength of SOC, we directly compare the full relativistic band structure with the scalar-relativistic one (without SOC). We notice that around -2.2 eV a sixfold degenerate crossing at the Γ point is split into a fourfold and a twofold crossing once SOC is included, with an energy separation of approximately 0.56 eV (not

shown). This roughly amounts to a SOC-induced splitting of about 0.28 eV.

A. Topological multifold crossings and Fermi arcs

The band structure of BeAu features multiple examples of exotic crossings, which are not encountered in conventional Weyl semimetals, and are enforced by the symmetries of the crystal. While conventional WPs are described by a local Hamiltonian which is adiabatically connected to $H_{\mathbf{k}} = \sigma \cdot \mathbf{k}$, the presence of additional crystalline symmetries allows the generalization to higher-dimensional intersections. Such objects will be described by a Hamiltonian of the form $H_{\mathbf{k}} = \mathbf{S} \cdot \mathbf{k}$ with $\mathbf{S} = (S_x, S_y, S_z)$ being some n -dimensional (iso)spin matrices.

B20 compounds have been shown to host fourfold degenerate crossings at the time-reversal-invariant momenta (TRIM) Γ and sixfold ones at R, with a chiral charge of -4 and $+4$, respectively [18,36–38]. Here, we find them at -0.4 eV (at Γ) and at -1.5 eV (at R), in agreement with Ref. [36]. We further confirm the value of the topological charge by explicitly integrating the Berry curvature over a small surface centered around such crossings. These ± 4 Weyl fermions give rise to four surface Fermi arcs connecting Γ to $\bar{M}$ – the projection of R onto a two-dimensional (2D) surface BZ. The arcs can be visualized by computing the surface spectral function on the (001) termination. Figure 2 shows the results for different energy cuts starting from the Fermi level (a) up to 0.2 eV above it (e). The best resolution of the arcs is achieved at higher energies, Fig. 2(e), where fewer bulk bands are present: very long states originating from $\bar{\Gamma}$ and following a complex trajectory culminate in a “spiraling” behavior near $\bar{M}$. Their connectivity becomes clear if the plot is extended to the neighboring BZ. On the contrary, at the Fermi level, the arcs strongly hybridize with the surrounding states, and they become hard to track.

To gain deeper insight into the physics of the arcs, we examine their evolution as a function of energy. We observe three key features, each marked by a different colored arrow in Fig. 2. Starting from 0.2 eV, the first feature appears around 0.15 eV: it corresponds to the opening of the circular surface states at the $\bar{X}$ point, the red arrow in panel (d). Simultaneously, the long arcs around $\bar{M}$ are pushed downward, signaling the onset of a connectivity exchange between the two. This process continues down to approximately 0.10 eV, where the inner circle around $\bar{X}$ also breaks open (blue arrow). At 0.06 eV, the arcs originally stemming from the right side of $\bar{\Gamma}$ are now attached to the spectral weight around $\bar{X}$, rather than connecting to $\bar{M}$. At this point, it is necessary to comment on the additional spectral weight near $\bar{X}$. These supplementary surface states also originate from the same Fermi arcs connecting $\bar{\Gamma}$ to $\bar{M}$: their strong dispersion in this compound causes them to cross the Fermi level multiple times. A similar behavior is theoretically predicted for GeRh [18], but here the effect appears to be significantly more pronounced. In panel (f), we also show the spin character of these surface states. We observe an avoided crossing along the $\bar{X}$ - $\bar{Y}$ direction: the less dispersive arcs with strong spin-down (red) components are “separated” by the more dispersive spin-up (blue) state.

Lastly, another connectivity exchange takes place around 0.10 eV, which we indicate with the green arrow in Figs. 2(b)

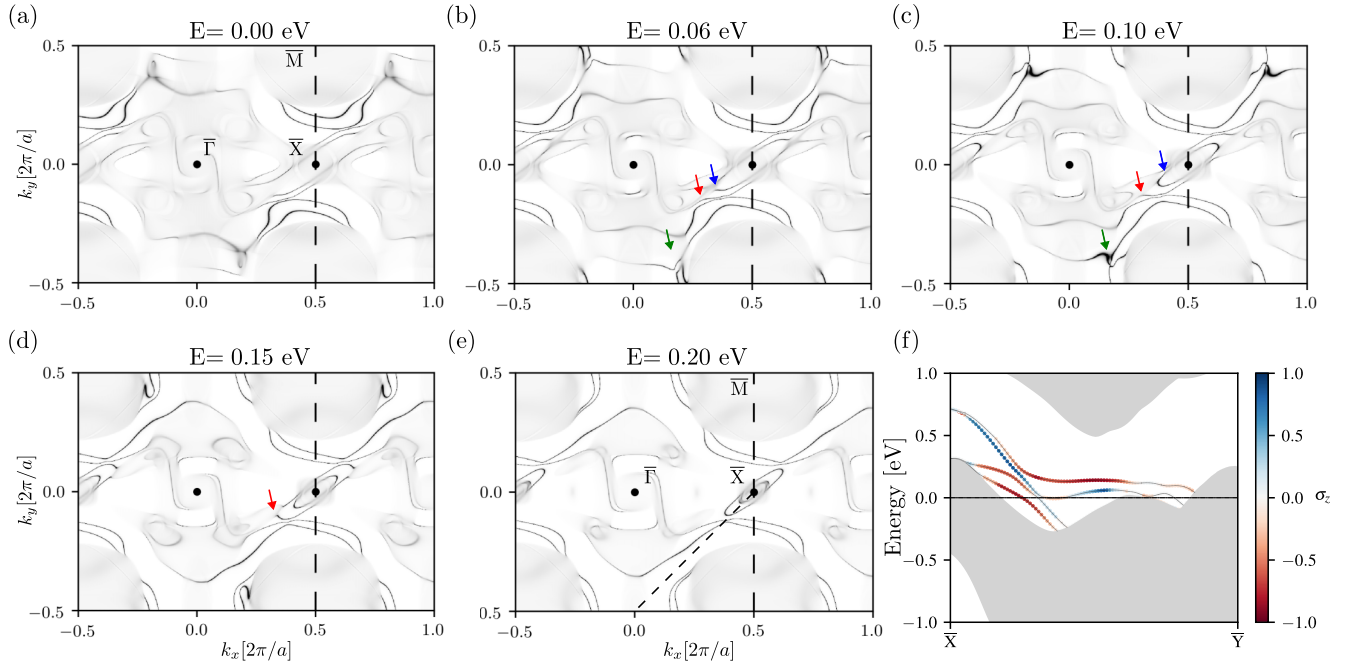


FIG. 2. Spectral function $A(\mathbf{k}, \omega)$ at fixed energy, evaluated at a depth of 10 Bohr radii (5.29 Å) for the (001) surface termination. In panel (a), $A(\mathbf{k}, \omega)$ is shown at the Fermi level, while panels (b)–(e) correspond to $\omega = 0.006, 0.10, 0.15$, and 0.2 eV, respectively. The red, green, and blue arrows highlight the change of connectivity between Fermi arcs, as discussed in the main text. Panel (f) displays the band structure of a ten-layer slab along the dashed path indicated in panel (e). Bulk states are shown in gray, while surface states are colored according to the expectation value of $\hat{S}_z$. We define a surface state as a band whose atomic weight on the first layer exceeds 30%. Surface states associated with the opposite termination are not shown.

and 2(c). This process is accompanied by the formation of a U-shaped structure with significant spectral weight, clearly visible in panel (c). An analogous behavior has also been reported to occur in RhSi, and it was found to realize type-II (surface) van Hove singularities [39]. It is therefore reasonable to expect the emergence of the same type of singularity in our case. Although we did not explore this aspect further in the present work, it certainly warrants further examination. Recent experimental [40] and theoretical [41–44] studies have shown that Fermi arcs can be highly sensitive to superconducting instabilities, leading to critical temperatures significantly higher than those observed in bulk crystals. Therefore, BeAu is a promising candidate to further investigate such a phenomenon, given the very large size of the arcs and the potential presence of van Hove singularities.

At this point, we observe that our surface state spectra are broadly consistent with the earlier results of Ref. [36], though some discrepancies are present. We attribute these differences to the choice of structural inputs for the DFT calculations (our use of experimentally determined lattice constants and Wyckoff positions versus the DFT-optimized structure in Ref. [36]) as well as the possibility of a different (unspecified) energy shift in the latter work.

In addition to the just-discussed $|C| = 4$ fermions, BeAu exhibits another type of multifold band crossing near the Fermi level, Fig. 1(f). This crossing is located at the TRIM point M, around 0.32 eV, and is referred to as a *double WP* or *charge-2 Dirac point* (DP). We will use the latter term

throughout. It comprises two overlapping WPs of the same chirality, resulting in a total topological charge of two. Its existence stems from the presence of screw-rotation symmetries and time-reversal symmetry ($\mathcal{T}$). As discussed later in Sec. III B, the combined action of $\tilde{C}_i$ and $\mathcal{T}$ enforces a two-fold degeneracy along the boundary of the BZ. Consequently, at the TRIM point M, a fourfold degeneracy must occur. A numerical analysis of the Wannier bands confirms that all crossings at the M point are indeed charge-2 DPs. The one closest to the Fermi level carries a topological charge of $C = -2$. Remarkably, the charge-2 DP at M does not give rise to additional surface Fermi arcs (see Sec. III B).

We conclude this section by discussing another degeneracy 3.5 eV below the Fermi level, which deserves mentioning as it constitutes the only known case where a band crossing can carry a topological charge of five. Originally, Bradlyn *et al.* [3] argued that the maximum Chern number permitted by crystalline symmetries originates from a fourfold crossing adiabatically connected to the spin-3/2 Hamiltonian, yielding $|C| = 4$ at half-filling. More recently, Alpin *et al.* [2] showed that in space groups 195 and 199, a fourfold crossing can exist that is *not* adiabatically connected to the spin-3/2 model, allowing Chern numbers of (3, -5, +5, +3) for the respective bands. However, the $C = \pm 5$ bands are always paired with the ones carrying $C = \mp 3$, so the net topological charge at half filling remains ± 2 , preserving the effective upper bound of $|C| = 4$. In Fig. 1(d), we color the band with $C = -5$ in purple and the band with $C = +3$

in green. A similar fourfold crossing occurs at even lower energies.

B. Unpaired Weyl crossings

Since periodicity requires that no net flux of Berry curvature crosses the surface of the BZ, nodes with equal and opposite chirality usually come in pairs, resulting in an overall net chirality of zero. To satisfy the condition of zero net Berry curvature flux across the BZ while permitting an isolated WP, a compensating source or sink of Berry curvature must exist. In certain chiral crystal structures, rather than a partner WP, this role is played by *nodal walls*: symmetry-protected nodal surfaces [13] that reside on the boundary of the BZ.

In such systems, the conventional picture of Weyl semimetals as stacks of 2D Chern insulators in reciprocal space becomes inadequate. Due to the presence of nodal surfaces at *all* BZ boundaries, no 2D slice of the three-dimensional BZ exhibits a full band gap. Consequently, the existence of a partner node is no longer required as the zero net-flux condition is met because of the nodal walls. Similarly, bulk-boundary correspondence breaks down, and such isolated WPs are not accompanied by topologically protected surface states [14].

In BeAu, the combination of time-reversal symmetry and skew rotations pins the nodal degeneracies at the edges of the BZ, hence the name nodal walls. This is because $(T\tilde{C}_i)^2 = e^{-ik_i \cdot \mathbf{t}_i}$, where $\mathbf{t}_i$ refers to a translation along i . Thus, Kramers' degeneracies are guaranteed at all $k_i = \pi$ planes since $(T\tilde{C}_i)^2 = -1$. These degeneracies can be seen in the band structure shown in Figs. 1(a) and 1(b), for example, along the M–X path. We marked them with red arrows for convenience. Note that as one moves away from the BZ boundary toward the interior (e.g., along Γ –M), the bands split again. It is important to stress that only the bands merging into these nodal walls can host unpaired WPs. For instance, the fourfold-degenerate fermions at Γ and R originate from bands not joined by nodal walls and thus behave as conventional pairs of Weyl nodes with associated surface Fermi arcs (Sec. III A).

The unpaired crossings can be conventional Weyls or even multifold fermions and can occur both at high-symmetry points—such as the charge-2 Dirac point at M—as well as at generic points in reciprocal space. To systematically explore their distribution, we performed a dense-mesh scan of the full BZ. Since there is no gap in the energy spectrum up to several eV from the Fermi level, we restricted our attention to the bands which intersect the Fermi level, identifying 81 WPs in the irreducible octant of the first BZ. We report in Fig. 3(c) the energy and positions of six unpaired WPs found within an energy window of 50 meV. Their projection onto the $k_x k_y$ -plane is also shown in panel (a) of the same figure.

In Fig. 3(b), we show the energy dependence of the crossings under applied pressure, which remains largely unchanged up to 3 GPa. This behavior aligns with the minimal variation observed in the DOS reported in the literature [29]. To determine the crystal structure at different pressures, we used the experimental curves for the lattice parameter a as a function of pressure from Ref. [29] and performed scalar-relativistic

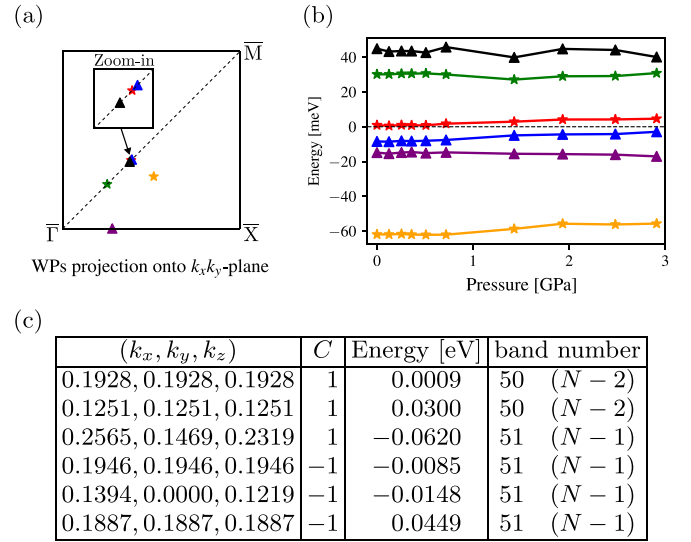


FIG. 3. Unpaired WPs at generic k points in the energy window of $\sim \pm 50$ meV around the Fermi level. (a) Projection onto the $k_z = 0$ plane of the WP positions belonging to the irreducible BZ. The asterisk (triangle) marks correspond to positive (negative) chirality. (b) WPs' energy dependence on external pressure. (c) Exact three-dimensional position (units of $2\pi/a$) of the nodes, with corresponding energy and chirality. The “band number” refers to our Wannier-projected Hamiltonian. We further label the same bands according to the order in which they appear at the fourfold fermion at Γ in Fig. 1(a): $N + 2$ corresponds to the highest eigenvalue.

symmetry-constrained relaxation of the atomic coordinates. This step was essential because even tiny changes in the crystal structure have a significant impact on the energy of the nodes. For example, the WP at -0.062 eV in our plot lies outside the energy range of ± 50 meV, however, using the value of $a_0 = 4.6699$ Å from Ref. [22] yields roughly -0.040 eV.

IV. FERMI SURFACE

In this section, we present a detailed analysis of the Fermi surface of BeAu, focusing on the topological charge carried by each part of the surface. Our motivation is twofold. First, the presence of unconventional crossings, we find, leads to Fermi sheets carrying unexpectedly high topological charge. Second, this quantity, also referred to as the Chern number of a sheet, together with the sign of the superconducting gap, characterizes the topology of a time-reversal invariant superconductor via Eq. (1) [16,17].

First of all, we present the Fermi surface in Fig. 4, which is highly complex, featuring numerous nested as well as intersecting sheets. We label each one increasingly from 1 to 12 in the order shown in the figure. In our notation, S_1 , S_3 , and S_5 each consist of three pockets, meaning they technically correspond to three distinct sheets for each plot. We group them together because they are symmetry-related. Around Γ , there are two small concentric and closed Fermi surfaces (S_7 and S_9), which become degenerate in the absence of SOC. An analogous situation arises near the R point, where, however, there are two pairs of intersecting surfaces ($S_8 \cup S_{10}$

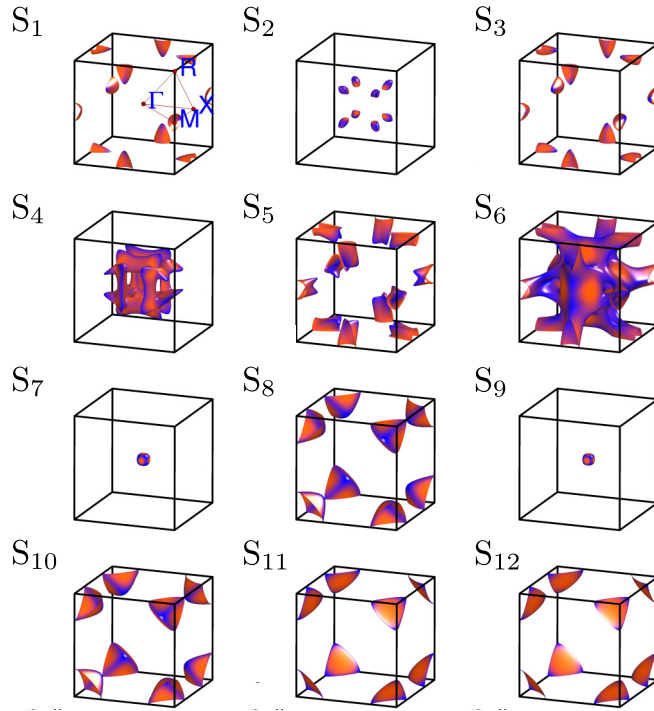


FIG. 4. All full-relativistic Fermi surfaces of BeAu computed with GGA and SOC with the de Haas–van Alphen module of FPLO. We used a $24 \times 24 \times 24$ k -mesh with an additional three bisections. The color gradient represents the Fermi velocity intensity (units not shown), ranging from low (blue) to high (orange) values.

and $S_{11} \cup S_{12}$). In this second case, the spin-orbit splitting is hardly noticeable.

To characterize the Chern number of each sheet, we perform a numerical integration to explicitly compute the flux,

$$C_i = \frac{1}{2\pi} \oint_{S_i} \Omega_i(\mathbf{k}) \cdot d^2\mathbf{k} = \frac{1}{2\pi} \oint_{S_i} \Omega_i(\mathbf{k}) \cdot \hat{\mathbf{n}}_i(\mathbf{k}) d^2k, \quad (2)$$

where S_i denotes the fully connected i -th part of the Fermi surface and $\Omega_i(\mathbf{k}) = \nabla_{\mathbf{k}} \times \langle u_{i,\mathbf{k}} | i\partial_{\mathbf{k}} | u_{i,\mathbf{k}} \rangle$ is the Berry curvature evaluated at the surface S_i . The vector $\hat{\mathbf{n}}_i$ specifies the normal direction of the surface element $d^2\mathbf{k}$, and it points along the direction of the Fermi velocity. We further recall that when multiple surfaces intersect, only the flux summed over all touching regions has physical significance and can be expected to be quantized.

In conventional Weyl semimetals, Eq. (2) can be evaluated implicitly, without explicit integration: a sheet enclosing a WP possesses a Chern number $|C| > 0$, whereas if no WPs are enclosed, the sheet has $C = 0$. This procedure, although still theoretically applicable here, becomes challenging due to the abundance of unpaired WPs and nodal surfaces.

To numerically perform the integration, we first obtain a fine triangulation of each surface S_i . Then the Berry curvature over each plaquette is obtained by averaging the values of $\Omega_i(\mathbf{k})$ at the three vertices. Finally, the normal vector $\hat{\mathbf{n}}_i$ is computed from the coordinates of the plaquettes' vertices with simple geometric rules. The main practical challenge in evaluating Eq. (2) arises for intersecting sheets. In such cases, two kinds of errors become relevant when sampling

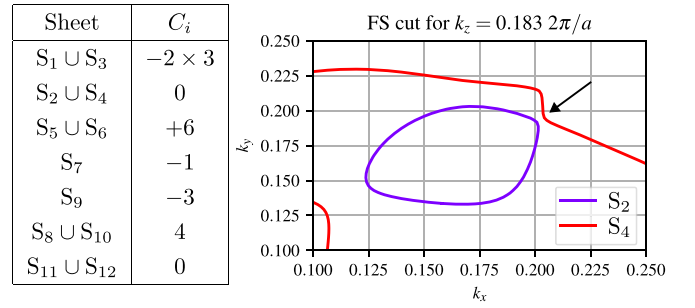


FIG. 5. On the left, the table summarizes the Fermi surface's Chern number as computed numerically from Eq. (2). In the first line, we make explicit that S_1 and S_3 have multiplicity of 3 because there are three symmetry-related M points. For bookkeeping purposes, we have grouped them together in all previous plots. In the second line, we decided to group S_2 and S_4 together because it was too demanding to computationally resolve the very small band gap (shown on the right).

the Fermi surfaces: (i) Wannier interpolation is not exact, and (ii) the Fermi surface is obtained by interpolating nearby points, so the k points assigned to a given surface S_i do not strictly lie on the isoenergy contour. This introduces a small shift $\delta\mathbf{k}$, which propagates into the surface integral. These errors are typically negligible since $\Omega_i(\mathbf{k})$ varies smoothly, but near band touchings, where $\Omega_i(\mathbf{k})$ can change rapidly, even small shifts accumulate. The more degeneracies present, the greater the computational effort required to control them. To address this issue, we can move slightly away from the Fermi level, where problematic degeneracies are absent or easier to resolve. For instance, this approach was used to determine the Chern number of S_6 , which was particularly challenging. At just 0.1 eV above the Fermi level, the surface splits into eight pockets centered around X, which we could evaluate separately and then sum their contributions. Finally, since gauge invariance requires $\sum_{i \in \text{FS}} C_i = 0$ [45], the chirality can still be inferred from the sum rule in the case one part of the Fermi surface fails to converge.

The results are summarized in the table in Fig. 5. Interestingly, the flux through the Fermi sheets around Γ , R, and M matches the value expected from the presence of multifold fermions sitting at the corresponding high-symmetry points, despite the presence of additional nearby crossings. The two sheets S_2 and S_4 present an extremely small gap, shown on the left of Fig. 5, which makes direct computation of the flux very sensitive to the mesh. Raising the energy slightly allows us to better resolve the gap, and we conclude (with a reasonable error of $\sim 0.37\%$) that both of them are trivial. However, for this conclusion to hold also at the Fermi level, we must know whether these bands intersect, not only at the Fermi level, but at all energies between 0 and 0.1 eV; otherwise, a possible redistribution of the topological charge is allowed. Given the very small size of the gap, the computational cost is high, and we decided not to pursue this any further. At present, we can say for certain that $C_2 + C_4 = 0$.

V. IMPLICATIONS FOR SUPERCONDUCTIVITY

Now that all sheets have been characterized, we can comment on the effect of an $s_{\pm}$ pairing state. To investigate the

consequences of a sign change in the gap function, Huang *et al.* [21] assumed a functional form $\Delta(\mathbf{k}) \sim \sum_i \cos(k_i)$. This choice is not unique since any basis of the trivial representation (A) can be chosen— $\cos(k_i)$ being the simplest. While this choice is suitable for their effective model, it need not hold for BeAu.

In the absence of further experimental inputs, it is difficult to propose a well-motivated alternative; however, what is important for the appearance of a topological superconducting phase is a sign change between different Fermi surfaces; this could happen in a multiband superconductor if the Fermi sheets involved are, for example, the ones at Γ and R. Under this assumption, our numerical evaluation of the Fermi surface's Chern number confirms that a topological superconducting phase with $\nu = 4$ can appear. We emphasize that numerically evaluating the surface Chern number was necessary due to the abundance of WPs located at generic positions, some even very close to Γ .

Although quite exotic, the presence of M pockets in theory enables the possibility of a different topological phase with $\nu = 6$. While such a phase may be unlikely to occur in BeAu due to the very small separation between S_6 and S_4 , similar electronic structures are common in B20 compounds, making this an intriguing possibility to consider.

As a concluding remark, looking at the atomic-resolved band structure in Fig. 1, we can also infer that S_5 and S_6 (centered at M) carry much more Be-character compared to the neighboring bands at the Fermi level. In Ref. [29], a simple model for the electron-phonon coupling involving only Be was proposed to explain the measured T_c . Given the good agreement with the experimental data, it is worth keeping in mind that the observed multigap formation could be linked to a nonuniform distribution of Be-character across the Fermi surface. In this case, however, a sign change between Γ and R becomes unlikely since the Γ and R points have a comparable degree of atomic hybridization. On the other hand, the possibility of a sign change between Γ and M remains, yielding the previously mentioned $\nu = 6$ topological phase. Such a phase was previously noted to be unlikely due to the small separation between the M pocket and other nearby Fermi surfaces, but it could be possible. Then, a more involved choice of the basis function for the irreducible representation A must be invoked to describe the $s_{\pm}$ gap function. Further investigation, i.e., k -resolved electron-phonon calculations, is therefore necessary.

VI. CONCLUSIONS

In this work, we employed DFT combined with Wannierization to characterize the electronic structure of the chiral Weyl semimetal BeAu. This material belongs to the B20 family of compounds, which is known for featuring multifold band degeneracies with high Chern numbers. We first reviewed the band structure of BeAu and identified the presence of $C = 4$ multifold fermions at the Γ and R points, consistent with previous literature. These band crossings lead to four extended Fermi arcs on the (001) surface termination, with extremely rich and complex connectivity behavior.

The nonsymmorphic skew-rotation symmetries inherent to space group $P2_13$ also permit the presence of unpaired WPs: topological crossings without counterparts of opposite chirality. In this case, the topological charge is compensated by nodal surfaces pinned at the BZ boundaries due to time-reversal symmetry. We identified many of these points close to the Fermi level and studied their behavior under hydrostatic pressure up to 3 GPa. We also pointed out that the charge-2 Dirac point at M represents an example of such isolated crossings.

Motivated by the experimental evidence for multigap superconductivity in BeAu and theoretical works on $s_{\pm}$ pairing in B20 compounds, we computed the Chern numbers of each Fermi surface sheet. We determined that the sheets surrounding the multifold fermions at Γ and R indeed carry Chern numbers of ± 4 , consistent with a $\nu = 4$ topological superconducting phase [21]. In the course of our analysis, we also discovered a large Fermi surface region carrying a Chern number of $+6$, the highest reported for a single Fermi sheet. This suggests the potential for a $\nu = 6$ topological phase, although its realization remains unlikely. However, similar Fermi surfaces are shared by many other B20 compounds (like the fellow superconductor RhGe), making our study of broader relevance. Additionally, independent of superconductivity, the existence of such high-Chern-number Fermi surfaces may have implications for transport responses beyond those seen in classical Weyl systems.

Finally, our atomic-projected band structure analysis revealed a significant difference in the orbital composition of the Fermi pocket around M compared to other states at the Fermi level, with the former showing a much stronger Be character. Given that superconductivity in BeAu is likely enhanced by Be-based electron-phonon coupling, this insight could be important for understanding the origin of its multigap superconducting behavior.

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DATA AVAILABILITY

Data and code available at the public repository [34].

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