Correlation-driven renormalization of topological features in the CeTX$_3$ series

Vsevolod Ivanov,1,* Xiangang Wan,2 and Sergey Y. Savrasov1,†
1Department of Physics, University of California, Davis, California 95616, USA
2Department of Physics, Nanjing University, Nanjing 210093, China

The precise nature of Cooper pairing in superconducting materials is determined by the underlying symmetry of the crystal lattice. In recent years, non-centrosymmetric superconductors have attracted particular interest, since the lack of inversion symmetry mixes spin singlet and triplet pairing states, and may allow the realization of topological superconductivity. The complex interplay of correlations and topology in these materials pose a particular challenge for numerical simulations. For this reason they are excluded from high-throughput searches for topological materials and instead treated on an individual basis. Here we study the electronic properties of the inversion-broken CeTX$_3$ heavy-fermion compounds, and find topological nodal lines as well as Dirac and Weyl points. The topological nodal lines have a significant effect on the Fermi surface spin structure that has not been considered in prior theoretical studies of the superconducting pairing. Our comprehensive treatment of this group of compounds is a critical first step in high-throughput searches of correlated topological materials.

Superconductivity in non-centrosymmetric compounds has received much attention due to their potential for hosting unconventional pairing states. The lack of inversion symmetry permits an antisymmetric spin-orbit coupling (ASOC) term in the Hamiltonian which splits the Fermi surface and introduces a mixing of spin-singlet and spin-triplet superconducting pairing states. The components of the mixed pairing state in these materials have a non-trivial momentum dependence that can result in accidental line nodes in the gap function, which is just one of the features of unconventional superconductivity (SC) in these systems.

The CeTX$_3$ (T = Co, Rh, Ir, X = Si, Ge) family of compounds crystallize in the BaNiSn$_3$-type structure ($I4mm$ space group, no. 107), which breaks spatial inversion symmetry (Fig.1). With the exception of paramagnetic CeCoSi$_3$, their low-temperature phases are antiferromagnetic (AF) at ambient pressure. Application of pressure suppresses the Néel temperature toward zero, where the magnetic ground state gives way to SC. The SC in this group exhibits many unconventional features, including upper critical fields $H_{c2}$ that far exceed the Pauli limiting field $H_p[T] \sim 1.86T_c[K]^{[1-8]}$ and have been suggested as evidence of an odd parity SC gap function. Recent work suggests that AF fluctuations play a role in the development of SC, indicating the importance of the spin structure to the unconventional physics in these compounds.

The lack of inversion symmetry is also a necessary ingredient for the existence of topological Weyl points. As the role of ASOC and absence of inversion symmetry in the development of the superconducting state is not well understood, we hope to shed some light by investigating the topological properties of this class of materials. Furthermore, the narrow Ce-4$f$ band is sensitive to temperature and pressure, Weyl points to be tuned without introduction of chemical or site disorder. This feature makes these heavy fermion materials promising candidates for the study of Weyl physics in the proximity of superconductivity and quantum criticality.

We study the electronic properties of these compounds within the framework of the full potential linear muffin-tin orbital method with spin-orbit coupling, using the experimentally measured lattice parameters [9–12]. The compounds are locked to the paramagnetic state to mimic the experimentally observed suppression of magnetism by pressure. The on-site interactions between the Ce-4$f$ electrons must be treated with special care, as the strong Coulomb repulsion dramatically narrows the bandwidth. We handle renormalization of quasiparticle bands through the LDA+Guzwiller (LDA+G) method, taking Hubbard $U$ values of 5eV and 6eV[13]. The method is described in more detail in Refs. [14–17]

In LDA+G, the double-counting potential must carefully be chosen to account for the Coulomb correction included in both the single-particle and interacting terms of the Hamiltonian. Specifically, for the electron self-energy correction, $\Sigma_\alpha(0) - V_{DC,\alpha}$, there are several options for the double counting potential $V_{DC,\alpha}$ [14]. One such option is to set $V_{DC,\alpha} = \Sigma_\alpha(0)$, which leaves the LDA Fermi surface (FS) intact. Another option is to average over orbital self-energies, $V_{DC,\alpha} = \frac{1}{N} \sum_\alpha N \Sigma_\alpha(0)$, allowing the
crystal-field modifications to be found self-consistently while keeping the average position of the correlated 4f orbitals fixed.

For the CeTX$_3$ compounds, the crystalline electric field (CEF) effect of the tetragonal symmetry lifts the degeneracy of the $J=5/2$ total angular momentum state, splitting it into three doublets. Magnetic susceptibility and inelastic neutron scattering experiments [18–21] have determined the ground state doublet to be $\Gamma_7^{(1)}$ with $\Gamma_6$ and $\Gamma_7^{(2)}$ slightly higher in energy. Our LDA calculation showed that the lowest energy doublet hybridizes with the four bands crossing the $E_f$ that are largely responsible for the shape of the FS. This is consistent with prior works that show qualitative agreement between the LDA Fermi surface and experimental de Haas-van Alphen (dHvA) measurements for CeRhSi$_3$ [12]. In order to best match the experimentally determined Fermi surfaces and mass enhancements we take a phenomenological approach and choose a hybrid double counting scheme which treats the lowest energy doublets independently from the others:

$$V_{DC,\beta} = \Sigma_{\beta}(0) \quad \text{for} \quad \beta = \Gamma_7^{(1)}, \Gamma_6$$

$$V_{DC,\alpha} = 0.1\text{Ry} + \frac{1}{N} \sum_{\alpha \neq \beta} \Sigma_{\alpha}(0) \quad \text{for all other states} \quad \alpha \neq \beta$$

where we additionally shift the remaining states upward by 0.1Ry, as has been previously done for Fermi surface calculations of isostructural LaTX$_3$ analogues which are used reference materials for the respective CeTX$_3$ compounds [22, 23]. The Fermi surfaces of the LaTX$_3$ series are presumed to be similar to those of CeTX$_3$ by previous works, due to the high degree of localization of Ce-4f electrons.

Our LDA+G procedure yields band-dependent quasiparticle residues $z_\alpha$, which are summarized in Table I. It is worth noting that the $\Gamma_7^{(2)}$ doublet has been determined to be the lowest lying state in CeRhSi$_3$ [23]. However, our calculations place the $\Gamma_7^{(1)}$ doublet at the lowest energy for all six isoelectronic compounds. The trends in the CeTX$_3$ series can be understood in terms of a Doniach phase diagram arising from competing RKKY and Kondo interactions [24]. The tuning parameter in the Doniach phase diagram is $|J_{ef}|N(0)$ where $J_{ef}$ is the magnetic exchange interaction and $N(0)$ is the density of states at the Fermi energy. Experimentally this parameter can be tuned by increasing pressure, which decreases the lattice volume. This results in a greater hybridization of the conduction and Ce-4f bands, decreasing the localization of the electrons. This localization can be seen directly from in the Néel temperatures of the compounds. The CeTGe$_3$ compounds have higher Néel temperatures ($T_N = 21$K, 14.6K, 8.7K vs. 0K, 1.8K, 5.0K for T = Co, Rh, Ir) than their Si counterparts, due to their larger lattice constants [9]. The Néel temperatures of CeRhSi$_3$ and CeIrSi$_3$ are suppressed to zero at relatively low pressures $P_c \sim 2$ GPa, indicating their proximity to the quantum critical point.

The $z_\alpha$ values we compute follow a decreasing trend with increasing lattice volumes, and qualitatively follow the experimental trend of larger quasiparticle masses as the weight of the transition metal atom increases. These imply a factor of $\sim 2-9$ increase in Sommerfield $\gamma$ values, but experimental measurements on CeTX$_3$ compounds in the high pressure paramagnetic state are not presently available.

For our choice of orbitals, the isoelectronic CeTX$_3$

\[ \begin{array}{cccccccc}
\text{TABLE I: Quasiparticle residues } z_\alpha & \text{for the two lowest energy doublets for the members of the CeTX}_3 \text{ series.} \\
\hline
\hline
z_{\text{LDA+G}} (U=5 \text{ eV}) & z_{\text{LDA+G}} (U=6 \text{ eV}) \\
\hline
\Gamma_7^{(1)} & \Gamma_6 & \Gamma_7^{(2)} & \Gamma_7^{(1)} & \Gamma_6 & \Gamma_7^{(2)} \\
\text{CeCoSi}_3 & 0.59 & 0.57 & 0.87 & 0.54 & 0.52 & 0.82 \\
\text{CeRhSi}_3 & 0.43 & 0.41 & 0.86 & 0.37 & 0.36 & 0.81 \\
\text{CeIrSi}_3 & 0.43 & 0.42 & 0.86 & 0.38 & 0.36 & 0.81 \\
\text{CeCoGe}_3 & 0.38 & 0.36 & 0.85 & 0.33 & 0.32 & 0.78 \\
\text{CeRhGe}_3 & 0.16 & 0.14 & 0.92 & 0.12 & 0.10 & 0.89 \\
\text{CeIrGe}_3 & 0.15 & 0.14 & 0.93 & 0.11 & 0.09 & 0.91 \\
\hline
\end{array} \]

\[ \text{FIG. 2: Band structure of CeCoGe}_3 \text{ calculated with} \]

\( (a) \) LDA and \( (b) \) LDA+G (below). The two lowest doublets, $\Gamma_7^{(1)}$ and $\Gamma_6$ are renormalized by correlations. The inset shows where the band-31 nodal line passes through the $xy$-plane, 0.1 eV below $E_f$.\]
compounds have 31 electrons, and the bands crossing the Fermi energy are numbered 29-32. These bands are predominantly Ce\textit{\text{-}4f} in character, with a minor contribution from the transition metal \textit{d}–orbitals away from the Fermi level. When Coulomb interactions are considered through the LDA+G calculation described above, their bandwidth is narrowed and the Fermi level is pinned to the lower doublet due to the increased density of states (Figure 2). We emphasize that while the particular number and shape of the topological features depend on the choice of doubling counting potential and magnitude of Hubbard-\textit{U}, their existence is guaranteed by symmetry and robust to correlations. Since the CeTX\textsubscript{3} compounds are isoelectronic, the general picture of their topological properties is the same, with each compound hosting different sets of particular features. To illustrate these various features, for the remainder of this work we will focus on describing the electronic properties of CeCoGe\textsubscript{3}, which hosts representative members of each type of topological feature found in the series, including Dirac points (DPs) \cite{25-30}, Weyl points (WPs) \cite{31-34}, and nodal lines (NLs) \cite{35-38}. 

In order to locate and confirm the topological features, we use a one shot method for data mining the bands \cite{39}. We divide the BZ into a k-grid of 20 \times 20 divisions, and compute the sum of Berry curvature fluxes through the surface of each k-cube in order to locate sources and sinks on an initial coarse grid. The locations of these topological points are subsequently refined by splitting each k-cube of the unit cell into a smaller grid of 4 \times 4 \times 4. The data mining procedure is repeated recursively on progressively smaller grids until the desired precision is achieved. This grid refinement allows us to resolve much finer details in the topologies of these materials.

First we will summarize the WPs in the BZ of CeCoGe\textsubscript{3}. We find two classes of WPs which are expected from the \textit{C}_{4\text{v}} point group symmetry. The first lies either in the \textit{k}_z = 0 or \textit{k}_z = 2\pi/c plane, and appears in sets of eight. The effect of the \textit{\sigma}_v and \textit{\sigma}_d mirror planes is to flip the charge of the WPs, so that WPs located at \((k_x, k_y, 0), (-k_x, -k_y, 0), (k_y, -k_x, 0),\) and \((-k_y, k_x, 0)\) have the same charge, while those found at \((-k_x, k_y, 0),\) \((k_x, -k_y, 0), (k_y, k_x, 0),\) and \((-k_y, -k_x, 0)\) have opposite charge. The second class of WPs comes in sets of 16, which respect the same symmetries about \textit{\sigma}_v and \textit{\sigma}_d and are additionally separated in the \textit{k}_z direction, with Weyls located at \((k_x, k_y, \pm k_z)\) having the same chirality. Table II summarizes the WP data for CeCoGe\textsubscript{3}, which is representative of the CeXT\textsubscript{3} series. For this compound we find seven (eight) non-equivalent Weyl points for the LDA (LDA+G) simulation.

In addition to WPs, the symmetry of the CeXT\textsubscript{3} structure allows for a number of other topologically protected features, including DPs, and NLs. Again, we focus on the features found in CeCoGe\textsubscript{3}, since the other isoelectronic CeTX\textsubscript{3} compounds host similar topological features. The numbers and types of features depend on the relative band positions determined by the CEF splitting in this family of compounds. Just as with the WPs, we reference each NL by the lower band number of the pair of bands forming the NL. The most striking topological structure in the BZ is the set of nodal lines emerging from the Dirac point in this material. The band inversion mechanism generating the Dirac point along the \textit{\Gamma} – \textit{Z} axis is similar to that responsible for the Dirac point in the inversion broken \textit{Cd}\textsubscript{\textit{3}}\textit{As}\textsubscript{\textit{2}} \cite{27}, which shares its \textit{C}_{\textit{4v}} point group symmetry. Along the \textit{\Gamma} – \textit{Z} direction, compatibility relations for the double group connect \textit{\Gamma}_7 \rightarrow \textit{\Lambda}_7 and \textit{\Gamma}_6 \rightarrow \textit{\Lambda}_6. When moving from \textit{\Gamma} towards \textit{Z} along the \textit{k}_z axis, the lowest lying \textit{\Lambda}_7 Kramer’s doublet switches with the \textit{\Lambda}_6 doublet. The Dirac point formed by the two doublets persists with the inclusion of band renormalizations, shifting from a position \textit{k}_z = 0.6442\textsubscript{\text{\AA}} in LDA to \textit{k}_z = 0.4285\textsubscript{\text{\AA}} in LDA+G, closer to the \textit{\Gamma} point, as shown in Figure 3.

Moving away from the \textit{\Gamma} – \textit{Z} axis within the \textit{\sigma}_v (\textit{\sigma}_d) mirror plane, compatibility relations dictate that the \textit{\Lambda}_6 and \textit{\Lambda}_7 doublets split into bands with \textit{\Sigma}_3/\Sigma_4 (\textit{\Delta}_3/\textit{\Delta}_4) irreducible representation. They can be distinguished by their mirror eigenvalue, with an eigenvalue of \(-i\) corresponding to \textit{\Sigma}_3/\textit{\Delta}_3 and \(i\) to \textit{\Sigma}_4/\textit{\Delta}_4. When bands belonging to different irreducible representations intersect within a mirror plane, they form a topologically

![FIG. 3: Band structures for CeCoGe\textsubscript{3} using (a) LDA, and (b) LDA+G. Bands are labeled with their character representations according to their mirror eigenvalue: \textit{\Sigma}_3/\textit{\Delta}_3 (blue) for \(-i\) and \textit{\Sigma}_4/\textit{\Delta}_4 (green) for \(i\) within the mirror planes. Along the \textit{\Gamma} – \textit{Z} line, doublets \textit{\Lambda}_6 (orange) and \textit{\Lambda}_7 (magenta) form a Dirac point. Nodal line crossings and Dirac points are indicated by black and red circles respectively.](image-url)
FIG. 4: Nodal lines in CeCoGe$_3$ from the touching of bands 29/30 (blue), bands 30/31 (green), and bands 31/32 (red), in the $\sigma_v$ and $\sigma_d$ mirror planes are plotted for LDA (a-c) and LDA+G (d-f). Labeled two dimensional projections of the nodal lines in LDA (a) and LDA+G (d) are provided for clarity, with the topological charge of each nodal line is indicated in parentheses. Three dimensional plots of LDA nodal lines A-G in the $\sigma_v$ plane (b) and LDA nodal lines H-O in the $\sigma_d$ plane (c). (e) shows the LDA+G nodal lines A-G in the $\sigma_v$ plane while (f) shows the LDA+G nodal lines H-L in the $\sigma_d$ plane.

TABLE II: The locations of non-equivalent Weyl points in the BZ of CeCoGe$_3$, given in units of $(2\pi/a, 2\pi/a, 2\pi/c)$. The Fermi energy is set to 0 eV. The band number refers to the band forming the lower half of the Weyl cone.

| Band | Location | Charge | $\# E$ (meV) | Band | Location | Charge | $\# E$ (meV) |
|------|----------|--------|--------------|------|----------|--------|--------------|
| 29   | (0.33860, 0.39343, 0.72781) | +1 | 16 -831.80 | 29   | (0.16695, 0.11984, 0.89380) | -1 | 16 -57.63 |
|      | (0.09700, 0.18704, 1.00000) | +1 | 8 -109.28 |      | (0.13255, 0.16138, 1.00000) | -1 | 8 -49.08 |
|      | (0.43351, 0.22853, 0.00000) | +1 | 8 -976.38 |
| 30   | (0.11761, 0.15192, 0.55611) | -1 | 16 -140.22 | 30   | (0.16312, 0.16831, 0.58602) | -1 | 16 -110.14 |
|      | (0.16536, 0.20827, 0.71579) | +1 | 16 -105.69 |
| 31   | (0.07098, 0.17299, 0.78441) | -1 | 16 +54.06 |
|      | (0.35171, 0.19625, 0.00000) | -1 | 8 +1.23 |
| 32   | (0.23461, 0.27132, 0.67584) | +1 | 16 +78.24 | 32   | (0.17352, 0.52586, 0.00000) | +1 | 8 +26.92 |
|      | (0.05697, 0.28539, 0.99636) | -1 | 16 +117.57 |      | (0.16677, 0.23615, 0.52961) | +1 | 16 +32.71 |
|      | (0.08304, 0.22061, 0.61719) | -1 | 16 +36.76 |

protected continuous line of degeneracy called a Weyl nodal line [40]. Such nodal lines are protected by the existence of mirror symmetry, and are robust against perturbations, surviving the introduction of correlations. We identify a total of 15 nodal lines in the LDA case, labeled NL-A through NL-O, and 12 nodal lines in LDA+G, labeled NL-A through NL-L. The nodal lines and their charges are shown in Figure 4. Additional details on the process of verifying the nodal lines can be found in the Supplementary Information.

We will now describe the nodal line features in CeCoGe$_3$ and how they are affected by band renormalizations. In LDA, four nodal lines emerge from the Dirac point, labeled NL-D, NL-G, and NL-N. NL-D loops back within the $Z - \Gamma - \Sigma (\sigma_v)$ plane (shown in green in Fig 1(b)), reemerging in the $Z - \Gamma - X (\sigma_d)$ plane (shown in magenta) as NL-O, which connects with itself through the top surface of the BZ as shown in Fig 4(b). NL-G instead curves downward, connecting with itself across the $xy$-plane.
The remaining NLs are either loops or extended lines spanning the entire BZ. The features lying close to the Fermi level are distorted dramatically by renormalization, while those that are lower in energy remain largely unchanged. Within the $\sigma_c$ plane, three band 29 nodal lines, NL-C, NL-D, and NL-E, merge and permute their connections in LDA+G. For instance, NL-C in LDA+G, which connects across $\Gamma - \Sigma$ and loops around to exit the BZ around the N point, is created from a merging of NL-C and NL-E found in LDA. A similar merging of NLs takes place in the $\sigma_y$ plane, where th NL-J loop merges with the left side of the NL-H loop in LDA to form NL-H in LDA+G which spans the entire BZ. The introduction of correlations completely destroys some features, such as NL-F of band 30 and NL-M, but also creates the new NL-F loop in band 31 in LDA+G. Despite having predominantly Ce-4$f$ character and lying close to the Fermi energy, NL-A and NL-K are surprisingly robust to renormalization. The remaining features, including the NL-B loop, NL-I, and NL-L remain mostly unchanged as Ce correlations are turned on, since they are lower in energy and have predominantly Co-3$d$ character.

As we have discussed, the renormalization of quasiparticle bands by correlations affects not only the momentum-space position of topological features, but also the energy at which they are located. Coulomb interactions dramatically reduce the Ce-4$f$ bandwidth which has the additional effect of pinning them to the Fermi energy due to the increased density of states. A consequence of this renormalization is that any topological features formed by the Ce-4$f$ bands will move closer to the Fermi energy, becoming more relevant to the material physics, particularly superconductivity.

We illustrate this by showing the renormalization of NL-I and the second WP residing in band 29 of CeCoGe$_3$ (Figure 5). Since the correlations only affect the energy and bandwidth of Ce-4$f$ bands, the effect on the nodal line can be understood by separately considering the lower (higher) energy part of the nodal line which has predominantly Co-3$d$ (Ce-4$f$) character. The effect of correlations is two-fold: first, the Ce-4$f$ part of the nodal line is shifted closer to the Fermi energy, and second the density of states is increased by the narrowing of the Ce-4$f$ band, pinning it to the Fermi level. As a result, the Fermi energy is shifted upward, and the Co-3$d$ part of the nodal line appears to shift down, since its energy remains relatively constant as the Co-3$d$ orbitals are unaffected by the correlations.

Likewise, the Weyl point located at $(0.097002 \pi, 0.18704 \pi, 1.0192 \pi)$ is formed from bands that hybridize strongly with the $\Gamma_2^{(1)}$ doublet near this momentum. The correlations introduced by LDA+G therefore cause a dramatic shift from 109 meV to 49 meV below the Fermi energy, and shift the Weyl point to a new momentum space position $(0.13255 \pi, 0.16138 \pi, 1.0192 \pi)$.

While superconductivity in the CeTX$_3$ compounds has been studied extensively, the exact mechanism of the spin pairing is still debated. More detailed discussions can be found in the literature [41–45], which we will briefly outline here. The superconducting pairing function $\Delta(k) = |\psi(k) + d(k) \cdot \tilde{\sigma}|^2 \delta_y$, is composed of even-parity scalar $\psi(k)$ and odd-parity vector $d(k)$ components, and the Pauli matrices $\tilde{\sigma} = \sigma_x, \sigma_y, \sigma_z$ act on the pseudospin basis states $|k, \uparrow\rangle$ and $|k, \downarrow\rangle$ [43]. The degeneracy between these two states is lifted by an inversion breaking ASOC term:

$$H_{\text{ASOC}} = \sum_k \sum_{\alpha\beta=\uparrow,\downarrow} \gamma(k) \cdot \tilde{\sigma}_{\alpha\beta} c_{k\alpha}^\dagger c_{k\beta}$$

where $c_{k\alpha}^\dagger$ ($c_{k\beta}$) are the creation (annihilation) operators for the pseudospin states. This term causes the states $|k, \uparrow\rangle$ and $|k, \downarrow\rangle$ to become non-degenerate, so that for sufficiently strong ASOC, the only available degenerate states must have opposite spin [45]. Then only the component of $d(k)$ parallel to $\gamma(k)$ is non-vanishing. Furthermore, the lack of inversion means there is no longer a symmetry to distinguish even and odd parity components, so $\psi(k)$ and $d(k)$ are free to mix. It has been proposed that anti-ferromagnetic spin-fluctuations near the superconducting transition drive the mixing of pairing states [41, 42].

It has also been suggested that CeRhSi$_3$ and CeIrSi$_3$ may be topological Weyl superconductors [43, 44], and indeed our present study has identified a number Weyl nodes in the energy dispersion. Type-I WPs have a spherical FS with an all-in/all-out hedgehog-like spin structures when the Fermi energy is located just above or

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**FIG. 5:** Renormalization of topological features in CeCoGe$_3$. (a) Renormalization of the $\sigma^{29}$ nodal line. The second Weyl point in band 29 (See Table II) plotted in (b) LDA and (c) LDA+G. The limits $k_A$, $k_B$, $k_C$, $k_D$ are the given by the Weyl point positions $\pm 0.1 \hat{k}_y$. 

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below the energy of the node. For opposite chirality WPs, spins located at time-reversal related momenta $\pm \mathbf{k}$ on their Fermi surfaces will be aligned, favoring a spin-triplet pairing. However, the WPs found in our calculations are Type-II, with their cones tilted below horizontal, resulting in hyperbolic FS that do not enclose the node. Their contribution to the FS topology is quite small, and most are too far from $E_f$ to be relevant for the superconducting physics, even when taking band renormalization into account. In fact, their relevance to the superconductivity in the CeTX$_3$ compounds is limited by the lattice symmetry. The anti-ferromagnetic state is destroyed by pressure before the onset of superconductivity, so time-reversal symmetry is preserved. Therefore Weyl nodes at $\pm \mathbf{k}$ would have equal chirality, meaning spins on their Fermi surfaces would be anti-parallel, and could not favor an equal-spin triplet pairing.

Instead we focus on the effect of topological NLs found in these compounds, which have occupy a significantly larger phase space. We emphasize that these topological NLs in the energy dispersion are distinct from the line nodes predicted to exist in the superconducting gap of these materials, and we consider their effect on the spin texture of the Fermi surface in the absence of any spin fluctuations or superconductivity. Figure 6 shows cross sections of the Fermi surface in the $z = 0$ plane for CeCoGe$_3$ in both LDA and LDA+G. We compare these with the commonly used tight-binding (TB) model with Rashba-type splitting that is used for theoretical studies of the CeTX$_3$ family:

$$H = \sum_k \epsilon_k c_k^\dagger c_k + \alpha \sum_k c_k^\dagger \gamma(k) \cdot \mathbf{\sigma} c_k$$  \hfill (4)

$$\gamma(k) = -2t_1(cos k_x + cos k_y) + 4t_2(cos k_x cos k_y) - 8t_3 cos(k_z/2) cos(k_y/2) cos(k_z)$$  \hfill (5)

where the parameters $(t_1, t_2, t_3, \alpha) = (1.0, 0.475, 0.3, 0.4)$ have been shown to reproduce the principal features of the LDA Fermi surface [41] (in our model, the magnitude of Rashba coupling $\alpha$ is doubled from the usual value of 0.2 for clarity). When compared with the TB model in Figure 6(a), our numerical simulations show a realignment of the Fermi surface spins beyond the usual Rashba coupling, as a consequence of the topological nodal lines near the Fermi energy. In LDA, the NL-M passes through the $xy$-plane very close to the Fermi energy, as can be seen from the intersecting surfaces concentric around the $X$ point in Fig 6(c). The topological charge enforces a reversal of the band spin texture when passing through the nodal line. In LDA+G correlations force the partial annihilation of the NL-M and NL-H nodal lines, leaving the NL-H as the only intersection of the bands in the $xy$-plane in LDA+G. However, the correlations do not prevent the spin reversal at the $\sigma_d$ planes, which originates from the point at which NL-H crosses the $xy$-plane in LDA+G, shown in the inset of Fig 6(d).

Our analysis shows that each nodal line found in the electronic structure can create a spin distortion that propagates to the FS, even when the nodal line is located far from the Fermi energy. This spin distortion causes a dramatic discontinuity in the spin structure at the mirror planes, in addition to helical spin structure introduced by Rashba ASOC. Crucially, prior studies of
superconductivity in the CeTX$_3$ compounds do not take into account the significant effect of this spin distortion.

In summary, we have performed simulations of superconducting compounds in the CeTX$_3$ series with LDA and LDA+G, choosing the double counting potential in such a way that reproduces the experimental Fermi surfaces. We characterized the topological properties of their energy dispersion finding WPs and NLs, which are renormalized close to the Fermi energy by the strong Coulomb interactions of the Ce$-4f$ orbitals. These topological features in turn affect the spin-structure at the Fermi surface in these materials and need to be carefully considered in future studies of the superconductivity pairing.

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* E-mail: vivanov@ucdavis.edu

1 E-mail: savrasov@physics.ucdavis.edu

[1] R. Settai, Y. Okuda, I. Sugitani, Y. nuki, T. D. Matsuda, Y. Haga, and H. Harima, International Journal of Modern Physics B 21, 3238 (2007), https://doi.org/10.1142/S0217979207044287.

[2] N. Kimura, K. Ito, K. Saitoh, Y. Umeda, H. Aoki, and T. Terashima, Phys. Rev. Lett. 95, 247004 (2005).

[3] F. Honda, I. Bonalde, K. Shimizu, S. Yoshiuchi, Y. Hirose, T. Nakamura, R. Settai, and Y. Ōnuki, Phys. Rev. B 81, 140507 (2010).

[4] I. Sugitani, Y. Okuda, H. Shishido, T. Yamada, A. Thamizhavel, E. Yamamoto, T. D. Matsuda, Y. Haga, T. Takeuchi, R. Settai, and Y. nuki, Journal of the Physical Society of Japan 75, 043703 (2006), https://doi.org/10.1143/JPSJ.75.043703.

[5] H. Wang, J. Guo, E. D. Bauer, V. A. Sidorov, H. Zhao, J. Zhang, Y. Zhou, Z. Wang, S. Cai, K. Yang, A. Li, X. Li, Y. Li, P. Sun, Y.-f. Yang, Q. Wu, T. Xiang, J. D. Thompson, and L. Sun, Phys. Rev. B 97, 064514 (2018).

[6] T. Kawai, M. Nakashima, Y. Okuda, H. Shishido, T. Shimoda, T. D. Matsuda, Y. Haga, T. Takeuchi, M. Hedo, Y. Uwatoko, R. Settai, and Y. nuki, Journal of the Physical Society of Japan 76, 166 (2007), https://doi.org/10.1143/JPSJS.76S1A.166.

[7] R. Settai, Y. Miyauuchi, T. Takeuchi, F. Ivy, I. Sheikin, and Y. nuki, Journal of the Physical Society of Japan 77, 073705 (2008), https://doi.org/10.1143/JPSJ.77.073705.

[8] N. Kimura, K. Ito, H. Aoki, and T. Terashima, Phys. Rev. Lett. 98, 197001 (2007).

[9] T. Kawai, H. Muranaka, M.-A. Measson, T. Shimoda, Y. Doi, T. D. Matsuda, Y. Haga, G. Knebel, G. Laperotot, D. Aoki, J. Flouquet, T. Takeuchi, R. Settai, and Y. nuki, Journal of the Physical Society of Japan 77, 064716 (2008), https://doi.org/10.1143/JPSJ.77.064716.

[10] A. D. Hillier, D. T. Adroja, P. Manuel, V. K. Anand, J. W. Taylor, K. A. McEwen, B. D. Rainford, and M. M. Koza, Phys. Rev. B 85, 134405 (2012).

[11] V. K. Pecharsky, O.-B. Hyun, and K. A. Gschneidner, Phys. Rev. B 47, 11839 (1993).

[12] T. Terashima, M. Kimata, S. Uji, T. Sugawara, N. Kimura, H. Aoki, and H. Harima, Phys. Rev. B 78, 205107 (2008).

[13] B. T. Thole, G. van der Laan, J. C. Fuggle, G. A. Sawatzky, R. C. Karnatak, and J.-M. Esteva, Phys. Rev. B 32, 5107 (1985).

[14] R. Dong, X. Wan, X. Dai, and S. Y. Savrasov, Phys. Rev. B 89, 165122 (2014).

[15] K. M. Ho, J. Schmalian, and C. Z. Wang, Phys. Rev. B 77, 073101 (2008).

[16] X. Deng, X. Dai, and Z. Fang, EPL (Europhysics Letters) 83, 37008 (2008).

[17] X. Deng, L. Wang, X. Dai, and Z. Fang, Phys. Rev. B 79, 075114 (2009).

[18] A. D. Hillier, D. T. Adroja, P. Manuel, V. K. Anand, J. W. Taylor, K. A. McEwen, B. D. Rainford, and M. M. Koza, Phys. Rev. B 85, 134405 (2012).

[19] Y. Okuda, Y. Miyauuchi, Y. Ida, Y. Takeda, C. Tonohiro, Y. Oduchi, T. Yamada, N. Dutcung, T. D. Matsuda, Y. Haga, T. Takeuchi, M. Hagiwara, K. Kindo, H. Harima, K. Sugiyama, R. Settai, and Y. nuki, Journal of the Physical Society of Japan 76, 044708 (2007), https://doi.org/10.1143/JPSJ.76.044708.

[20] M. Smidman, D. T. Adroja, A. D. Hillier, L. C. Chapon, J. W. Taylor, K. A. Anand, R. P. Singh, M. R. Lees, E. A. Goremychkin, M. M. Koza, V. V. Krishnamurthy, D. M. Paul, and G. Balakrishnan, Phys. Rev. B 88, 134416 (2013).

[21] V. K. Anand, A. D. Hillier, D. T. Adroja, D. D. Khalyavin, P. Manuel, G. Andre, S. Rols, and M. M. Koza, Phys. Rev. B 97, 184422 (2018).

[22] A. Thamizhavel, H. Shishido, Y. Okuda, H. Harima, T. D. Matsuda, Y. Haga, R. Settai, and Y. nuki, Journal of the Physical Society of Japan 75, 044711 (2006), https://doi.org/10.1143/JPSJ.75.044711.

[23] Y. Muro, M. Ishikawa, K. Hirota, Z. Hiroi, N. Takeda, N. Kimura, and H. Aoki, Journal of the Physical Society of Japan 76, 033706 (2007), https://doi.org/10.1143/JPSJ.76.033706.

[24] S. Doniach, “Phase diagram for the kondo lattice,” in Valence Instabilities and Related Narrow-Band Phenomena, edited by R. D. Parks (Springer US, Boston, MA, 1977) pp. 169–176.

[25] S. M. Young, S. Zaeheer, J. C. Y. Teo, C. L. Kane, E. J. Mele, and A. M. Rappe, Phys. Rev. Lett. 108, 140405 (2012).

[26] Z. Wang, Y. Sun, X.-Q. Chen, C. Franchini, G. Xu, H. Weng, X. Dai, and Z. Fang, Phys. Rev. B 85, 195320 (2012).

[27] Z. Wang, H. Weng, Q. Wu, X. Dai, and Z. Fang, Phys. Rev. B 88, 125427 (2013).

[28] B.-J. Yang and N. Nagaosa, Nature Communications 5, 4898 (2014).

[29] Q. D. Gibson, L. M. Schoop, L. Muechler, L. S. Xie, M. Hirschberger, N. P. Ong, R. Car, and R. J. Cava, Phys. Rev. B 91, 205128 (2015).

[30] Y. Du, B. Wan, D. Wang, L. Sheng, C.-G. Duan, and X. Wan, Scientific Reports 5, 14423 (2015).

[31] X. Wan, A. M. Turner, A. Vishwanath, and S. Y. Savrasov, Phys. Rev. B 83, 205101 (2011).

[32] H. Weng, C. Fang, Z. Fang, B. A. Bernevig, and X. Dai, Phys. Rev. X 5, 011029 (2015).
[33] S.-M. Huang, S.-Y. Xu, I. Belopolski, C.-C. Lee, G. Chang, B. Wang, N. Alidoust, G. Bian, M. Neupane, C. Zhang, S. Jia, A. Bansil, H. Lin, and M. Z. Hasan, Nature Communications 6, 7373 (2015).
[34] A. A. Soluyanov, D. Gresch, Z. Wang, Q. Wu, M. Troyer, X. Dai, and B. A. Bernevig, Nature 527, 495 (2015).
[35] A. A. Burkov, M. D. Hook, and L. Balents, Phys. Rev. B 84, 235126 (2011).
[36] R. Yu, H. Weng, Z. Fang, X. Dai, and X. Hu, Phys. Rev. Lett. 115, 036807 (2015).
[37] Y. Kim, B. J. Wieder, C. L. Kane, and A. M. Rappe, Phys. Rev. Lett. 115, 036806 (2015).
[38] Y. Du, F. Tang, D. Wang, L. Sheng, E.-j. Kan, C.-G. Duan, S. Y. Savrasov, and X. Wan, npj Quantum Materials 2, 3 (2017).
[39] V. Ivanov and S. Y. Savrasov, Phys. Rev. B 99, 125124 (2019).
[40] C. Fang, H. Weng, X. Dai, and Z. Fang, Chinese Physics B 25, 117106 (2016).
[41] Y. Tada, N. Kawakami, and S. Fujimoto, Journal of the Physical Society of Japan 77, 054707 (2008), https://doi.org/10.1143/JPSJ.77.054707.
[42] Y. Tada, N. Kawakami, and S. Fujimoto, Phys. Rev. B 81, 104506 (2010).
[43] A. Daido and Y. Yanase, Phys. Rev. B 94, 054519 (2016).
[44] T. Yoshida and Y. Yanase, Phys. Rev. B 93, 054504 (2016).
[45] M. Smidman, M. B. Salamon, H. Q. Yuan, and D. F. Agterberg, Reports on Progress in Physics 80, 036501 (2017).