Electronic correlation effect on nontrivial topological fermions in CoSi

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Abstract. The present study has been carried out to understand the effect of electronic correlations on the recently found fermions in CoSi. For which the spectral functions of bulk and (001) surface of CoSi have been investigated using DFT + DMFT advanced methodology at $T = 100$ K with and without inclusion of spin–orbit coupling (SOC). The Co $d_{xz}$ + $d_{yz}$ and $d_{z^2}$ bands seem to contribute at threefold degenerate $\Gamma$ point. On the other hand, fourfold degenerate $R$ point seems to possess maximum of Co $d_{x^2-y^2}$ + $d_{xy}$ orbitals and minimum of $d_{xz}$ + $d_{yz}$ orbitals. However, SOC and electronic correlations appear to modify the nature of bands involved at $\Gamma$ point. DFT + DMFT calculations for the bulk states have shown one extra hole pocket at $M$ point. Incoherent features seem to be possessed by mostly Co $d_{xz}$ + $d_{yz}$ orbitals in the spectra of bulk CoSi. The existence of both coherent and incoherent features indicates the presence of quasiparticle–quasiparticle (QP–QP) interactions which is eventually affecting the lifetime ($\tau$) of exotic fermionic QPs. For instance, the calculated $\tau$ for QPs at $\omega \sim -3$ and $-186$ mev are found to be $\sim 10^{-9}$ s and $\sim 10^{-12}$ s, respectively, when SOC is not considered. However, $G_0W_0$ corrections have shown $\tau$ for spin-1 fermionic QP at $\Gamma$ to be infinite while for double Weyl fermionic QP at $R$ point to be $\sim 10^{-12}$ s. Their effective masses ($m^*$) have also been calculated as $\sim 1.60$ and $1.64$ at $\Gamma$ and $R$ points, respectively. Furthermore, the spectral functions at $T = 100$ K of (001) surface have also shown both coherent and incoherent features. Consequently, at $\omega = 0$ for surface states, $\tau$ has been calculated of the order $\sim 10^{-8}$ s for both without SOC and with SOC inclusions.

1 Introduction

For past few decades, there has been a quest for novel fermionic particles other than Dirac, Majorana, and Weyl in the field of elementary-particle physics [1]. Interestingly, in the recent years, condensed matter systems have also shown the existence of various exotic fermionic quasiparticles (QPs) such as two-dimensional (2D) Dirac fermions in graphene [2], helical Dirac fermions at the surface of three-dimensional (3D) topological insulators [3,4], Majorana fermions in topological superconductors [5–9], and Dirac semimetals and Weyl semimetals [10–19]. Exploration of these kind of fermionic QPs is very important due to their potential of applicability in the field of electronics and information technology.

Following the history, Herring investigated the degeneracies occur in electronic band structures, and he noted that even in the absence of any symmetry, one could obtain a twofold degeneracy in a 3D solid [20]. The dispersion in the vicinity of these degeneracy points (the band-crossing/touching points) is generally linear and resembles the Weyl equation which lacks the Lorentz invariance [20]. Such band touching points in solids as discovered by Herring are then named as Weyl nodes/points by Wan et al. [20,21]. The key feature of determining such band touching points is the degeneracy of bands which in turn is realized by symmetry. The Weyl points can be found in 3D solids only when either time-reversal or inversion symmetries are broken. On other hand, when both the symmetries are present, the possibility of a twofold degeneracy at a Weyl point in the spectrum gets excluded. This rather produces a fourfold degeneracy at band-crossing points which is also termed as Dirac node [19]. Thus, at the band touching points, Weyl fermions have twofold degeneracy and the Dirac fermions have fourfold degeneracy. However, recent studies have shown new types of massless fermions with many-fold degeneracies in solid state systems which have no analogs in high-energy physics [22–27]. These newly found fermions appear in crystals with specific space group symmetries [28]. For example, spin-1 fermion with threefold degeneracy carrying ±2 topological charge, spin-3/2 Rarita–Schwinger–Weyl fermion (RSW) with fourfold degeneracy carrying ±4 topological charge [28–30], double Weyl fermions

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with $\pm 2$ topological charge [31–33], and double spin-1 fermion with sixfold degeneracy [22]. Interestingly, these newly found fermions are predicted to be seen in topological chiral systems like transition-metal (TM) monosilicides such as XSi ($X = \text{Co, Rh, Fe}$) [28,32,34–38]. Among these, the present work is mainly focused onto CoSi for the study.

First-principle band structure calculations over CoSi and its angle-resolved photo-emission spectroscopic study (ARPES) have already predicted and shown it to be topological chiral systems [28,35–37,39]; belongs to the family of CoGe, RhSi, and RhGe with P2$\text{\textsubscript{1}}$3 as spacegroup [40]. The 3D band structure calculations without spin–orbit coupling (SOC) for CoSi have predicted two types of unconventional linear band-crossing points, one at $\Gamma$ with threefold degeneracy corresponding to spin-1 fermion and other at $R$ with fourfold degeneracy corresponding to double Weyl fermion [28,39]. Tang et al. have also shown that topological surface states (SS) become apparent from the projections of spin-1 excitation and a double Weyl fermion at $\Gamma$ and $R$ [28]. Moreover, when band structure calculations are performed with SOC consideration; resulted into two separate crossing points both at $\Gamma$ and $R$, respectively [28]. Thus, recent works are mainly focused into the prediction and realizing the existence of unconventional chiral fermions and their associated fermi-arc states for CoSi material theoretically and experimentally [28,35–37,39,41–43].

All these theoretical works have been carried out at the density functional theory (DFT) level. In the independent-electron picture QPs possess infinite lifetime. Thus, in those DFT studies, the newly found QPs have infinite lifetime, and the informations of their interactions are missed out. It is well known that in solids, QP–QP interactions broaden the single non-interacting particle $\delta$-function peaks, renormalize them, and redistribute the spectral weight between the coherent and incoherent structures. These incoherent structures often called Satellites or sidebands. Thus, it is important to characterize these exotic fermionic QPs in interacting picture and which can be achieved using beyond DFT method, i.e., dynamical mean field theory (DMFT). For dealing many electron problems and strong correlation effects in solids, DFT + DMFT is a sophisticated formulation [44–47], has been used recently [48–51]. This formulation deals with local impurity problem, where self-energy ($\Sigma(\omega)$) contains all the information regarding QP excitations [52]. However, these days, $GW$ calculations are also performed for getting the QP’s informations, but this method is computationally very costly. This $GW$ approximation is a many-body perturbation theory as developed by Hedin [53]. Here, $G$ stands for one electron Green’s function and $W$ stands for screened Coulomb interaction. In this theory, the self-energy ($\Sigma$) is a function of both crystal momentum ($k$) and frequency ($\omega$), and can calculate $\Sigma$ of QPs at any $k$-point in Brillouin zone (BZ). However, in this theory, one-shot $GW$ ($G_0W_0$) is well established which is a all electron $GW$-based technique, and not much computationally demanding [39,49]. Thus, usage of these two advanced methodologies will provide an insight of these fermions’ behavior inside strongly correlated electron system like CoSi. This kind of investigation is required, because a bridge between the existing unconventional chiral fermions with non-trivial topology and the electronic correlations is missing. The present work is motivated with this thought, and accordingly, we have revisited the already found topological chiral fermions in CoSi with the usage of advanced formulations.

Considering the above-mentioned aspects, we have studied the spectral functions for both bulk and (001) surface of CoSi using DFT + DMFT methodology at $T = 100 \text{ K}$ [54] with and without SOC inclusions. All the new fermions are observed at $\Gamma$ and $R$ points as expected yet one extra hole pocket is found at $M$ points. The Co $d_{xz} + d_{yz}$ and $d_{z^2}$ bands appear to contribute at threefold degenerate $\Gamma$ point. On the contrary, four-fold degenerate $R$ point seems to posses mixture of Co $d_{xz} + d_{yz}$ orbitals and $d_{x^2-y^2} + d_{xy}$ orbitals (where the latter one has maximum contribution). Mostly, Co $d_{xz} + d_{yz}$ orbitals seem to only contributing to incoherent weights in the spectra of bulk CoSi. As DFT + DMFT calculations have shown the presence of both coherent and incoherent features in spectra. Suggesting the lifetime ($\tau$) of the newly found fermions to be affected due to QP–QP interactions. For instance, the calculated $\tau$ for QPs at $\omega \sim -3$ and $-186 \text{ mev}$ are found to be $\sim 10^{-9}$ $s$ and $\sim 10^{-12}$ $s$, respectively, when SOC is not considered. However, $G_0W_0$ corrections have given $\tau$ for spin-1 fermionic QP at $\Gamma$ to be infinite while for double-weyl fermionic QP at $R$ point to be $\sim 10^{-12}$ s. Similarly, $\tau$ is calculated for other new fermionic QPs as found when SOC is considered using both DFT + DMFT and $G_0W_0$ methods. Moreover, at $T = 100 \text{ K}$, the spectral functions of (001) surface have also shown the existence of both coherent and incoherent features. Accordingly, at $\omega = 0$, $\tau$ has been evaluated which is of the same order $\sim 10^{-8}$ $s$ for both noc SOC and SOC considerations.

### 2 Computational details

The DFT-based electronic structure calculations have been performed using WIEN2k code [55]. This code is based on full-potential plane wave (FP-LAPW) method. PBEsol is taken as exchange functional for the calculations [56]. The experimentally observed crystal structure is taken from the literature [57]. 2.18 and 1.84 Bohr are the muffin-tin sphere radii for Co and Si sites, respectively, with $10^{-3}$ as charge convergence. 21x21x21 mesh grid size in BZ has been used for the bulk states calculations.

Next, single-site DFT + DMFT calculations have been performed using the code as implemented by Haule et al. [54] which is interfaced with WIEN2k code [55]. This DMFT code provides stationary free energies at finite temperatures [58]. Accordingly, DMFT calculations are carried out for 100 K temperature, and all
the calculations are performed fully self-consistently in the impurity levels and electronic charge density. The auxiliary impurity problem is solved using a continuous-time quantum Monte Carlo impurity solver here [59]. Exact double-counting (DC) scheme as proposed by Haule has been used here [60]. For the formulation of exact DC, he proposed a new method of calculating the exact overlap between the DMFT and a band structure methods such as DFT. It is achieved quite generally using the Luttinger–Ward functional [60]. More informations regarding this can be found at Ref. [46,54,60–62]. Full 3d orbitals of Co are treated at DMFT level. The density–density form of Coulomb repulsion has been employed here with the usage of self-consistently calculated values of \(U(4.5\, \text{eV})\) and \(J(0.94\, \text{eV})\) from our previous work [63]. The analytical continuation as needed for obtaining the self-energy on the real-axis maximum entropy method is used here [64].

Furthermore, to calculate the QP energies at particular \(k\)-points, 1 shot-GW \((G_0W_0)\) calculations are performed using the Questaal package [65]. This code is based on full-potential linearized muffin-tin orbital (FP-LMTO) method [66,67]. In this code, \(G_0W_0\) calculations are perturbations to a DFT calculation. They are simpler than quasiparticle self-consistent GW calculations, because only the diagonal part of \(\Sigma\) is normally calculated (this is an approximation) and they use only one self-energy is calculated (single iteration). Its GW implementation description can be found in Ref. [68]. Here again, the exchange functional and the muffin-tin sphere radii for Co and Si sites are kept same as mentioned above.10 \(\times 10 \times 10\) mesh grid for DFT calculations in BZ, while \(4 \times 4 \times 4\) mesh grid for the self-energy in \(G_0W_0\) calculations have been used.

Finally, the surface states of 001 surface are calculated at both DFT and DMFT levels. For this, a slab of thickness 33.54 Bohr has been taken containing 32 atoms. To minimize the interactions between two consecutive slabs, a 30 Bohr vacuum has been provided along \(k_z\) direction. Moreover, SOC is considered in all the calculations.

3 Results and discussion

3.1 Bulk band structure without spin–orbit coupling

Figure 1a illustrates the crystalline lattice structure of CoSi which crystallizes in a cubic lattice with non-symmorphic space group \(P2_13\) and lacks inversion symmetry. Here, Co and Si atoms are located at 4a sites with position coordinates at \((x,x,x)\) in a unit cell with \(x_{Co} = 0.140\) and \(x_{Si} = 0.843\). The corresponding Brillouin zone (BZ) along high-symmetric lines is shown in Fig. 1b, which is a cube with the \(\Gamma\)-point at the center, \(R\) points at the vertices, \(X\)-points at the centers of the faces, and \(M\)-points at the centers of the edges of the cube. The projected BZ of 001 surface along high-symmetric lines \((M - \Gamma - X)\) is shown in Fig. 1c.

Figure 2a shows the bulk band structure as obtained from DFT and Fig. 2b shows momentum-resolved many-body spectral function calculated within DFT + DMFT at temperature \((T) = 100\, \text{K}\), along high-symmetric \(k\)-directions in the energy window \(-0.5 \leq \omega \leq 0.2\, \text{eV}\). Further for better visualizations, the enlarged pictures of bulk band structures corresponding to the band-crossings found at \(\Gamma\) and \(R\) points in BZ are plotted in Fig. 2c–f as obtained from DFT and DMFT, respectively. In all the figures, the bands are further resolved into Co 3d orbitals. Accordingly, red color is set for \(d_{xz} - d_{yz}\), blue color is set for \(d_{x^2 - y^2} + d_{xy}\), and green color is set for \(d_{x^2 - y^2}\). All of these figures are plotted without SOC considerations. Here, it is also important to note that only 100 K is chosen on the basis of previous report [48]. Previously, it has been seen that temperature has minimal effect on the value of imaginary part of self-energy. Considering this, it is expected to observe the same behavior of quasiparticle lifetime as a function of temperature. Before stating the differences between the two plots; here, it is important to understand that there is a difference in studying the electronic dispersion curves as generated from DFT and DFT + DMFT methods. Generally, the spectral function \((A(k,\omega))\) is defined as \(A(k,\omega) = -\text{Im}G^R(k,\omega)/\pi\) where \(G^R(k,\omega)\) is the retarded Green’s function for the interacting electron system. \(G^R(k,\omega) = 1/(\omega - \epsilon_0(k) - \Sigma(k,\omega))\), where \(\Sigma(k,\omega)\) is the self-energy term in which all the interaction effects are contained. However, for the independent-electron picture (non-interacting system), \(\Sigma(k,\omega)\) term is zero and \((A(k,\omega))\) has a \(\delta\)-function peak at \(\omega = \epsilon_0(k)\). As DFT represents the non-interacting electron picture, here, \(A(k,\omega) = \delta(\omega - \epsilon_0(k))\). This non-interacting system case can be observed from the
spectral function obtained from DFT, where the electron possesses one distinct energy ($\epsilon_0(k)$) at a given $k$ point for some $n$th band where $n$ and $k$ act as a good quantum numbers. On the other hand, within DFT + DMFT, for a single band, the $A(k, \omega)$ is written as given in Eq. 1 [52]:

$$A(k, \omega) = \frac{1}{\pi} \frac{-\text{Im}\Sigma(k, \omega)}{[\omega + \mu - \epsilon_0(k) - \text{Re}\Sigma(k, \omega)]^2 + [-\text{Im}\Sigma(k, \omega)]^2}.,$$

where $\omega$ is real frequency, $\mu$ is the chemical potential, $\epsilon_0(k)$ is the single particle energy with crystal momentum ($k$), and $\text{Im}\Sigma(k, \omega)$ is the imaginary part and $\text{Re}\Sigma(k, \omega)$ real part of the self-energy, respectively. This $A(k, \omega)$ will have one major peak with some finite width and rest spectrum will have broadened structures. The major peak is associated with DFT $\delta$ peak with broadened shape at an energy position $(\omega = \epsilon_0(k) + \text{Re}\Sigma(k, \omega) - \mu)$; this peak will correspond to coherent weight. The rest broadened structures in the spectrum will be corresponded to incoherent weight. Now, when this spectrum is seen on a larger scale with large numbers of $n$ and $k$, the whole spectrum then has smeared attributions with sharp dispersive lines. The sharp dispersive lines are then associated with coherent weights (states with large lifetime) and smeared features of the spectrum with incoherent weights (states with shorter lifetime).

Here, it is important to note that in this study, single-site DFT + DMFT calculations have been performed, and thus, the self-energy will have only $\omega$ dependence. $\text{Im}\Sigma(\omega)$ contains the information regarding the lifetime of QPs. Larger is the value of $\text{Im}\Sigma(\omega)$ lesser will be the lifetime of QPs. However, to get a better picture of the lifetime of QPs at particular $k$-point, $G_0W_0$ calculations are performed in this study. It is because $GW$ approximations work on the entire crystal, and thus, within this approximation, $k$ is a good quantum number. Further with the knowledge of $\text{Re}\Sigma(\omega)$, the effective band mass renormalization parameter $(m^* = 1 - d\text{Re}\Sigma/[d\omega|_{\omega=0}]$ and QP weight $(Z = 1/m^*)$ can also be calculated. This $m^*$ provides the information of the renormalization of bands due to the inclusion of Coulomb interactions, resulting in a spectral weight transfer between the incoherent and coherent states. Generally, $Z$’s value remains $< 1$ and positive for the interacting electron systems instead of $1$ which is for the case of non-interacting system. Thus, more closer the value of $Z$ to $1$, lesser will be the transfer of spectral weight from coherent states to incoherent states. Finally, by following the Eq. 1, the lifetime ($\tau$) of QP can be calculated as $\tau \approx h / \text{FWHM}$; where FWHM is full width half maximum [69], and in Eq. 1, FWHM is $\approx 2 \text{Im}\Sigma(k, \omega)$.

Now, on the basis of above explanations, the two figures [Fig. 2a, b] are compared. First, well-defined dispersive lines in Fig. 2a, while in Fig. 2b, smeared features (blurred bluish and pinkish color) with sharp dispersive lines (white color) are observed in the provided energy window. Here, the sharp dispersive lines are representing the coherent QPs (larger lifetime), while the blurred ones are representing the incoherent states. The incoherency of spectra seems to become large when $\omega \leq -0.2$ eV. This can also be observed from Fig. 3a, where the value of $\text{Im}\Sigma(\omega)$ is negligibly small till $\omega \sim -0.2$ eV, whereas its value started increasing when $\omega \leq -0.2$ eV for all the three $3d$ components of Co. Second, in Fig. 2a, one hole pocket around $\Gamma$ point and one electron pocket around $R$ point are observed. On the other hand in Fig. 2b, two hole pockets are seen around $\Gamma$ and $M$ points, respectively, and one electron pocket at $R$ point. The hole-like bands near the Fermi energy at $\Gamma$ point and electron-like bands at $R$ points are in good agreement with ARPES report [36]. Regarding extra hole pockets at $M$ points, seem to be generated due to electronic correlations. However, ab-initio calculations as performed by Sanchez et al. have reported hole pocket at $M$ point which is unlike Tang et
al.’s report [28,35]. This suggests the urge of observing hole pocket at M point which is also addressed by Xu et al. [70]. Thus, this motivates to carry out ARPES study for finding more hole-like bands near $E_F$ at M points. Furthermore, the hole-like band at M points appears to be white in color with pinkish and bluish blurred out-lining in Fig. 2b; indicating that the hole-like band is having all the 5 flavors of Co 3d orbitals where the QP is possessing coherent weight, whereas Co $d_{x^2-y^2} + d_{xy}$ and $d_{xz} + d_{yz}$ orbitals seem to be possessed by QPs with incoherent weights. This result is unlike DFT observation where maximum of Co $d_{xz} + d_{yz}$ orbitals than $d_{x^2-y^2} + d_{xy}$ orbitals seem to contribute at M point in Fig. 2a.

Third, two band-crossing points are found at Γ and R points in both figures. At Γ point, two linear and one flat bands are involved, while at R point, four linear bands are involved which is also evident from Fig. 2c–f. However, in moving from Fig. 2a–b, there are shifts in energy positions of band-crossing points found at Γ and R. For instance, the Γ and R points have shifted from ~ 12 to ~ 3 meV and from ~ 194 to ~ 186 meV, respectively. In the above discussion, this is seen that for a single band the DFT δ peak is supposed to be positioned at $\omega = \varepsilon_0(k) + \text{Re} \Sigma(\omega) - \mu$ when studied within DMFT. However, in the case of multi-band picture, for a single ω, the value of ReΣ(ω) will have contributions from all bands. Moreover, the expression has μ dependence and within DMFT chemical potential will be derived. With respect to the chemical potential when the states will be filled then considering their weights, there is a possibility of energy shifts there too. Consequently, there will be a collective effect which may lead to positive or negative shifts in the energetics of bands and in general which may have k dependence. This appears to be the reason for observing the shifts of energy positions of bands within DMFT when compared with DFT ones.

Next, at DFT level, it is found that the threefold degenerate bands at Γ point have mainly Co $d_{xz}$ + $d_{yz}$ orbitals contribution, whereas fourfold degenerate bands at R point have maximum contribution from Co $d_{xz}$ + $d_{yz}$ orbitals and minimum from Co $d_{x^2-y^2} + d_{xy}$ orbitals, and thus, no contribution from Co $d_{xz}$ orbital in the given energy window (also evident from Fig. 2c, d). However, at DMFT level from Fig. 2b, it is seen that the threefold degenerate bands at Γ point are shown in cyan color (mixture of green and blue color) suggesting to have almost equal mixture of Co $d_{xz}$ + $d_{yz}$ and $d_{xz}$ orbitals which are also coherent (sharp feature) in nature. Yet, bluish smeared feature is also observed which is suggesting the contribution from only Co $d_{xz}$ + $d_{yz}$ around the Γ point, whereas the tails of the flat band are in pink color (mixture of red and blue) further suggesting mixture of Co $d_{x^2-y^2} + d_{xy}$ and $d_{xz}$ + $d_{yz}$ orbitals (can be seen in Fig. 2e).

Then, moving to fourfold degenerate bands at R point in Fig. 2a, red color seems to be more prominent than blue color. Clearly, showing the maximum flavor of Co $d_{x^2-y^2} + d_{xy}$ orbitals than $d_{xz}$ + $d_{yz}$ orbitals. However, in Fig. 2b, the electronic correlations seem to change the flavors again. Now, the bands at R point are in pinkish color with an outlining of bluish color suggesting the contributions from both Co $d_{x^2-y^2} + d_{xy}$ and $d_{xz}$ + $d_{yz}$ orbitals, and the QPs present here with these bands character seem to have incoherent weights. Yet, white colored bands are also seen at R point suggesting all the five 3d orbitals to be present there with almost equal contribution, and here, the QPs are expected to have coherent weights. For better understanding all these observations, one can look into Fig. 2c–e. Moreover, considering Fig. 2e, one can observe that at around Γ point, the hole pocket seem to exist just in Γ − R direction but not in Γ − M direction which is unlike DFT result. Hence, from all these observations, one can understand the nature of bands involved in these band-crossing points in an interacting picture. All these results are unlike DFT results clearly showing the effect of correlations on these QPs. Moreover, these threefold degenerate and fourfold degenerate band-crossing points at DFT level are in good agreement with other theoretical and experimental works [28,35–37].

### 3.2 Fermionic quasiparticles lifetime

The threefold degeneracy has been associated with spin-1 fermion, while the other fourfold degeneracy with double Weyl fermion. In Fig. 2b as the band-crossing points, Γ and R are lying in the range of $−0.2 \leq \omega \leq 0.2$ eV where the value of ImΣ(ω) is negligibly small, this suggests that spin-1 and double Weyl fermionic QPs seem to have coherent weights (larger lifetime due to QP–QP interactions which is otherwise infinite in the case of non-interacting system). Consequently, at $\omega \sim −3$ meV and $\omega \sim −186$ meV, the $\tau$ of QPs are evaluated as $\sim 10^{-9}$ s and $\sim 10^{-12}$ s, respectively. However, $G_0W_0$ corrections have shown that the ImΣ is almost zero for spin-1 fermionic QP at Γ point indicating its $\tau$ to be almost infinite, while $\tau$ of double Weyl fermionic QP at R point is found to be $\sim 10^{-12}$ s. Furthermore, the effective masses of QPs ($m^*$ values) as calculated from DFT + DMFT and $G_0W_0$ methods are given in Table 1. Following the table, almost equal values of $m^*$ seem to be possessed by all the three components of Co 3d orbital at both ω’s. Indicating that the QPs have become heavier due to electronic correlations, and further suggesting spectral weight transfers between coherent and incoherent states of these components in almost equal amount. This behavior can also be witnessed from Fig. 3a where all the three components of Co 3d orbitals have negligible value of $\text{Im} \Sigma(\omega)$ around the $E_F$. Finally, the $m^*$ values as calculated from DFT + DMFT method at both ω are containing the informations of both spin-1 and double Weyl fermionic QPs with QPs available at other k points due to the fact that ImΣ depends upon only ω. Although, this is not the case with $m^*$ values as evaluated from $G_0W_0$ method due to the fact that here ImΣ is a function of both k and ω. Thus, 1.60 and 1.64 are the effective masses of spin-1 and double Weyl fermionic QPs found at Γ and R points, respectively.
Table 1  Calculated $m^*$ for different $\omega$ corresponding to $\Gamma$ and $R$ points without SOC consideration at $T = 100$ K as evaluated from DFT + DMFT method for three orbital components of Co $3d$ orbital and other at $T = 0$ K as evaluated from $G_0W_0$ method, respectively. Different $\omega$ values are corresponding to energy positions of band-crossing points as obtained from Fig. 2b

| $k$-points ($\omega$ (meV)) | Orbital component (DFT + DMFT) | $G_0W_0$ |
|-----------------------------|--------------------------------|----------|
|                             | $z^2/m^*$                      | $z^2 - y^2/xy$ | $xz/yz/m^*$ | $m^*$ |
| $\Gamma$ ($\omega \sim -3$) | 1.16                           | 1.19      | 1.20      | 1.60 |
| $R$ ($\omega \sim -186$)   | 1.16                           | 1.20      | 1.23      | 1.64 |

Fig. 3  Imaginary part of self-energy ($\text{Im}\Sigma(\omega)$) as a function of energy at $T = 100$ K for three components of $3d$ orbitals of Co a without SOC and b with SOC. Zero energy corresponds to the Fermi level (dotted line)

3.3 Bulk band structure with spin–orbit coupling

To see the effect of SOC on the spectral function in the presence of electronic correlations, Fig. 4a–f is plotted. In Fig. 4a, the DFT obtained bulk band structure, and in Fig 4b, momentum-resolved many-body spectral function calculated within DFT + DMFT at $T = 100$ K are shown. Both of them are plotted along high-symmetric $k$-directions for the energy window $-0.5 \leq \omega \leq 0.2$ eV. Here again, the enlarged pictures of bulk band structures corresponding to the band-crossings found at $\Gamma$ and $R$ points in BZ are plotted in Fig. 4c–f as obtained from DFT and DMFT methods, respectively, with further depiction of band character. At DFT level, SOC has been found to split all the bands by 1–2 meV. Yet, there is no change in the band character involved in exotic fermions found at special $k$-points. However, substantial changes are found in the character of bands involved at $\Gamma$ point only in an

Fig. 4  a Bulk band structure of CoSi with SOC consideration as obtained from DFT calculation, and b momentum-resolved many-body spectral function with spin–orbit coupling consideration at $T = 100$ K obtained from DFT + DMFT. c–f Bulk band structures corresponding to $\Gamma$ and $R$ points obtained from DFT and DFT + DMFT methods, respectively. Zero energy represents the Fermi level
interacting picture. Accordingly, the dispersion plot is again resolved into Co $3d$ orbitals in Fig. 4b in the given energy window.

It has been shown that for space group 198 (to which CoSi belongs) in the absence of inversion symmetry, SOC inclusion tends to lift the double degeneracy at non time-reversal (TR) invariant $k$-points, while at TR invariant $k$-points, the double degeneracy stays protected [22]. $M$ being TR invariant $k$-point, the double degeneracy remains intact. Yet, extra hole pockets at $M$ point, they have got enhanced and the energy positions of the bands at $M$ have shifted from $\sim - 16$ to 23 meV in Fig. 4b. However, no change in the band character at $M$ points is found. However, at $\Gamma$-point, the sixfold degeneracy has split into two crossing points one with twofold and other with fourfold degeneracy in Fig. 4a, b. The twofold degeneracy is associated with spin-1/2 Weyl fermion, while fourfold degeneracy is associated with spin-3/2 RSW fermion. On moving from Fig. 4a, b, changes in energy positions of these band-crossing points at $\Gamma$ and $R$ points have been found again as expected.

At $\Gamma$, the fourfold degenerate point has moved from $\sim 30$ to 4 meV in Fig. 4b, while the twofold degenerate point has moved from $\sim - 23$ to 40 meV in Fig. 4b. Moreover, out of fourfold degenerate bands, three linear bands are seen in cyan color, while one almost linear band is in pinkish color (evident from Fig. 4e). Suggesting those 3 bands containing mixture of Co $d_{xz}$ and $d_{yz}$ characters, while one remaining band consists of both Co $d_{z^2}$ and $d_{xy}$ characters. Thus, the QPs present at $\Gamma$ point possessing mixture of Co $d_{z^2}$ and $d_{xy}$ and Co $d_{x^2-y^2}$ and $d_{xy}$ and $d_{xz} + d_{yz}$ orbitals seem to be coherent in nature (due to its sharpness). Similarly, for other twofold degenerate bands at $\Gamma$ point, here again, both the bands seem to have Co $d_{z^2}$ and $d_{xz} + d_{yz}$ characters. However, in the entire region of Fig. 4e, bluish colored smearing can be seen indicating the QPs found at $\Gamma$ consisting of Co $d_{xz} + d_{yz}$ orbitals seem to have incoherent weights. This bluish smearing has increased direct effect of spin–orbit coupling.

Considering Fig. 4c, two more linear band-crossing points (the marked ones) appear to be created at $\sim -6$ meV in $\Gamma - M$ direction, while another at $\sim -4$ meV in $\Gamma - R$ direction, respectively. However, other flat band-crossing point has been created at $\sim 16$ meV in $\Gamma - R$ direction. These two band-crossing points in $\Gamma - R$ direction are recognized as type-I Weyl fermion, while band-crossing point in $\Gamma - M$ direction is recognized as type-II Weyl fermion by Tang et al. [28]. It is said that type-I Weyl semimetals have point-like Fermi surface at Weyl points, whereas in type-II due to high tilting of the Weyl cone, the Weyl points exist at the boundaries between electron and hole pockets in the Fermi surface. For more informations, one can refer to [71,72]. At DFT level, these new types of Weyl fermions seem to have just Co $d_{xz} + d_{yz}$ character only, while this is not the case with DMFT result. Interestingly, on observing Fig. 4e, the inclusion of SOC and Coulomb interactions has been found to change the curvatures of flat bands with enhanced incoherent weights. This has resulted in hole pockets in both the directions $\Gamma - M$ and $\Gamma - R$ unlike Fig. 2e. Furthermore, other band-crossing points can be clearly seen in Fig. 4e, though their energy positions has shifted. Likewise, the two linear band-crossing points are located at $\sim - 17.4$ meV in $\Gamma - M$ direction and at $\sim - 19.3$ meV in $\Gamma - R$ direction in Fig. 4e. The flat band-crossing is found to be shifted to $\sim 5$ meV in $\Gamma - R$ direction in Fig. 4e.

Next, at $R$-point in Fig. 4a, b, a crossing point with sixfold degeneracy is found, which corresponds to double spin-1 excitations and its energy position has shifted from $\sim -186$ to $-182$ meV. However, two bands become degenerate just few energies below sixfold degenerate point and this too has shifted from $\sim -220$ to $-207$ meV in Fig. 4b. In Fig. 4f, the bands at $R$ point can be seen in white color suggesting not much changes in its band character, whereas the incoherency of the spectrum has increased. Considering Fig. 4d, two more linear band-crossing points are observed which are twofold degenerate in $\Gamma - R$ direction where one is located at $\sim -205$ meV and other is at $\sim -262$ meV, respectively. These two band-crossing points are identified as type-II Weyl fermion by Tang et al. [28]. In Fig. 4f, the other twofold linear band-crossings in $\Gamma - R$ direction are now located at $\sim -204$ meV and $\sim -250$ meV where features are again highly smeared. The features being highly smeared suggesting the existence of incoherent weights, indicating larger QP–QP interactions. Besides, seeing the white color bands in these type-II Weyl fermions, it can be concluded that these fermions contain all the five flavors of Co $3d$ orbitals with coherent weight.

### 3.4 Fermionic quasiparticles lifetime

In Fig. 4b, the incoherent features seem to be enhanced at both band-crossing points where $\omega < -0.2$ eV, and this can be validated from Fig. 3b where Im$\Sigma(\omega)$ is negligibly small. Existence of incoherent features at both $\Gamma$ and $R$ points suggests the interactions between the QPs; affecting their lifetime. Thus, at $\omega \sim 4$ and $-40$ meV, their $\tau \sim 10^{-9}$ s, while at $\omega \sim -182$ and $-207$ meV, their $\tau \sim 10^{-12}$ s. It is already known that an exact information of newly fermionic QPs interactions at specific $k$-points cannot be retrieved from DFT + DMFT calculations; for which $G_0W_0$ corrections calculated the $\tau$ of newly fermionic QPs available at $\Gamma$ and $R$ points as $\sim 10^{-9}$ s and $\sim 10^{-11}$ s, respectively. Here again, the $m^*$ values as calculated from DFT + DMFT and $G_0W_0$ methods are given in Table 2. From the table, it can be seen that DFT + DMFT has shown almost same effective masses of the QPs $\sim 1.20$. However, $G_0W_0$ has shown effective masses of spin-1/2 Weyl fermionic and spin-3/2 RSW fermionic QPs at $\Gamma$ to be same $\sim 1.6$, whereas double spin-1 fermionic QPs found at $R$ point to have effective mass of $\sim 1.67$. 
Table 2  Calculated $m^*$ for $\Gamma$ and $R$ points with SOC consideration at $T = 100$ K as evaluated from DFT + DMFT method for three orbital components of Co 3$d$ orbital and other at $T=0$ K as evaluated from $G_0W_0$ method, respectively. Different $\omega$ values are corresponding to energy positions of band-crossing points as obtained from Fig. 4b.

| $k$-point (\(\omega\) (meV)) | Orbital component (DFT + DMFT) | $G_0W_0$ |
|-----------------------------|-------------------------------|----------|
|                             | $z^2$                         | $x^2 - y^2/xy$ | $xz/yz$ | $m^*$ |
| $\Gamma$ (\(\omega \sim 4\)) | 1.18                          | 1.20      | 1.20    | 1.60 |
| $\Gamma$ (\(\omega \sim -40\)) | 1.18                          | 1.19      | 1.20    | 1.61 |
| $R$ (\(\omega \sim -182\)) | 1.18                          | 1.20      | 1.20    | 1.67 |
| $R$ (\(\omega \sim -207\)) | 1.19                          | 1.20      | 1.20    | 1.64 |

Fig. 5 Band structure of (001) surface of CoSi obtained from DFT both for without SOC inclusion when the slab thickness is a 33.54 Bohr and b 100.64 Bohr. The surface states are marked with solid lines (red color) and bulk states are marked with dashed lines (black color). Zero energy represents the Fermi level. Elliptical markings are shown for explanation purpose.

3.5 Topological surface states

In the last part of discussion and results, the effects of slab thickness and electronic correlations over the surface states (SS) when projected to the (001) surface of CoSi along high symmetry lines $\overline{M} - \Gamma - \overline{X}$ are discussed. Generally, it is said that hole and electron pockets in the bulk are possessed by nontrivial topology and due to which SS can be observed on the side surface [28]. Based on this, the SS are expected to be observed on the side surface (001) of CoSi due to the presence of electron and hole pockets in the bulk at $\Gamma$ and $R$ points in Figs. 2a, b and 4a, b. Accordingly, Fig. 5a, b is plotted, showing the surface band structures as calculated from DFT for (001) surface without
SOC consideration when slab thicknesses are (a) 33.54 Bohr and (b) 100.64 Bohr, respectively. Two surface bands (I and II) have been found at the projections of bulk states at Γ and R points in Fig. 5a, b, respectively, marked in solid lines (red color). This is similar to the electronic spectra for (001) surface as reported by Tang et al. [28]. For explaining the changes occurred in the SS while going from Fig. 5a, b, a few elliptical markings have been numbered in the plots. In Fig. 5a, it is observed that at marking 1 surface bands I and II, both are crossing the Fermi level (EF) separately, while at marking 2, only surface band II has crossed the EF. Next, at marking 3, both surface bands I and II merged together and cross the EF as a single band, whereas in marking 4, none of them crosses the EF and remain below the EF. Finally, at marking 5 only surface band I crosses the Γ point at ~ 166 meV. Moving to Fig. 5b, it is found that at marking 1, both surface bands merged together crosses the EF as single band, while at marking 2, this time, the surface band I slightly shifts above the EF. Then, at marking 3, both the surface bands crosses the EF separately. At marking 4, surface band II cross over the EF, while surface band I remains below the EF. This time at marking 5 and marking 6 both surface bands I and II crosses the Γ at ~ 47 meV and 130 meV, respectively. All these points suggest that there are no more changes on the number of crossings at EF of the surface bands I and II. Based on this, it can be concluded that SS are not much affected with the change in slab thickness in the energy window of −50 ≤ ω ≤ 50 meV. Furthermore, the momentum-resolved many-body spectral functions for (001) surface are also plotted for with and without SOC effect at T = 100 K in Fig. 6a, b, respectively. Due to high computational cost, for the calculation of surface states from DFT + DMFT method, the slab thickness with 33.54 Bohr is only chosen. On looking at Fig. 6a, b, one can find that here again the surface states seem to emerge from the projections of bulk states at Γ and R points as expected. In Figs. 6a and 6b, both the surface bands appear to cross the EF at marking 4 (as marked in Fig. 5) unlike DFT results. Furthermore, on moving from Fig. 6a, b, the incoherency of the spectrum (smeared features) appears to enhance specifically in the region −0.1 ≤ ω ≤ −0.2 eV. This suggests that these surface states are interacting and due to which their lifetime is also affected. For instance, from Fig. 6a, b at ω = 0, the τ ∼ 10−8 s.

4 Conclusion

In this work, the electronic spectra of bulk and (001) surface of CoSi have been studied using advanced DFT + DMFT method at T = 100 K for both with and without SOC inclusions, respectively. From the DFT + DMFT calculations for the bulk states, one extra hole pocket is found at M points in BZ. All the newly discovered fermions are observed similar to other theoretical and experimental reports. Threefold degenerate Γ point seems to possess a mixture of Co dxy + dyz and dz2 orbitals. However, maximum of Co dxy + dyz and dz2 orbitals and minimum of dxy + dyz orbitals appear to contribute at fourfold degenerate R point. These results are unlike DFT results where there is no contribution from Co dz2 orbital at both Γ and R points. However, SOC and electronic correlations found to modify the band character especially at Γ point. Now, the QPs possess both the mixture of Co dxy + dyz and dz2 orbitals and Co dxy − dyz and dz2 orbitals. Dispersion curves of bulk CoSi as obtained from DFT + DMFT method have shown that incoherent features seem to be possessed by mostly Co dxy + dz2 orbitals. The existence of both coherent and incoherent features in the dispersion curves of Bulk CoSi has suggested the QP–QP interactions, further is resulting into affecting their lifetime. For example, τ for QPs at ω ∼ −30 and −186 mev are found to be ~ 10−9 s and ~ 10−12 s, respectively, when SOC is not considered. However, G0W0 has given τ for spin-1 fermionic QP at Γ as infinite, while for double Weyl fermionic QP at R point as ~ 10−12 s. Their effective masses are also calculated by using G0W0 method as ~ 1.60 and 1.64. Similarly, the τ and m∗ values of other fermionic QPs are also calculated using both DFT + DMFT and G0W0 method under SOC inclusion. Furthermore, at T = 100 K, the electronic spectra of (001) surface have also shown both coherent and incoherent features. Consequently, for both noc SOC and SOC inclusions at ω = 0, τ ∼ 10−8 s has been calculated.

Author contributions

SKP is solely responsible for the problem formulation and direction. PD has performed the numerical simulations. Under the guidance of SKP, PD has analyzed the data and wrote the manuscript.

Data Availability Statement This manuscript has no associated data or the data will not be deposited. [Author’s comment: First of all, this is a purely computational work, and all the data (processed) related to this work is already provided in the form of figures and tables within this article. Only raw data are kept with the authors. Because of this, we chose this option of no data/data will not be deposited while submitting the manuscript.]

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