Explicit View of Multi-Weyl Character

A set of hopping amplitudes was obtained from Wannier functions based on 48 atomic orbitals, viz. Bi 6p, P 3p, Ca 4s, 3d. The 4 bands crossings along Γ-Z as shown in Fig. 1a are reproduced by hopping amplitudes extending to nine neighbour unit cells. Fig. 1b-1e show energy dispersion perpendicular to \( \hat{z} \) for each of the four degenerate points, where two are seen to be multi-Weyls (Fig. 1b and 1c), i.e. dispersion is linear along \( \hat{z} \) but quadratic in directions perpendicular to \( \hat{z} \). This behavior is also seen in other Dirac semimetals, eg. Na\(_3\)Bi. The tight binding scheme can be extended to obtained a 4 \( \times \) 4 model Hamiltonian through \( k \cdot p \) expansion at \( \Gamma \) point. However, since the Weyl points do not occur at small \( k \), such an abbreviated expansion cannot reproduce a realiable description for the band crossings.
FIG. 1: Band structures obtained from the hopping-parameters up to nine neighbouring cells (six is minimum number of cells for the resulting bands to be reasonable). (a) The energy bands along Γ-Z shows four degenerate points where two are multi-Weyl points. (b)-(e) Energy dispersion perpendicular to $\hat{z}$ at $k_{x,j} = 0.032$ (left point), 0.039 (right point), 0.037 (bottom point) and 0.034 (top point), in units of ($\frac{\pi}{c}$).