

# Valley-polarized Quantum Anomalous Hall and Topological Metal Phase in Rashba induced pseudospin-1 lattice

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We study the topological properties of Rashba spin-orbit coupling and exchange coupling induced pseudospin-1 system Dice lattice under the influence of a staggered electric potential and magnetization. The band structure and topological phases of the system are investigated and compared with pseudospin- $\frac{1}{2}$  system honeycomb lattice. Under individual influence of the staggered electric field and magnetization, the system undergoes a distinct phase transition: (i) a staggered electric potential drives the system from a quantum anomalous Hall ( $C_n = 2$ ) to a valley polarized quantum anomalous Hall phase ( $C_n = -1$ ) associated with edge modes with a flip in the chirality; while (ii) a staggered magnetization changes the system to a topological metal associated with unconventional antichiral edge bands, from a topological insulator. These results are further supported by calculations of the Chern numbers, Hall conductance, zigzag, and armchair edge states. Our findings enhance the understanding of new topological phases in the 2D pseudospin-1 system and open up a new platform to explore the anti-chiral edge states.

## I. INTRODUCTION

Two-dimensional (2D) materials with band structures possessing a non-trivial topology have gained enormous research interest since they were first introduced by Haldane [1] that showed the quantized Hall conductance in the absence of an external magnetic field, which is known as the Quantum Anomalous Hall effect (QAH) and was later experimentally realized [2–4]. Essentially, it is achieved by breaking the time-reversal symmetry (TRS) using a complete next-nearest-neighbor hopping with opposite phases for two different sublattices in the Honeycomb structure [1]. In 2005, Kane and Mele ingeniously introduced a model that preserves time-reversal symmetry induced by strong intrinsic spin-orbit coupling (ISOC) [5, 6]. It shows the quantum spin Hall (QSH) effect, and host helical edge states are protected by time-reversal symmetry and characterized by a  $Z_2$  topological invariant. As the QAH and QSH phase display dissipationless edge states and topological currents that are extremely robust against disorder effects [7], they constitute a very attractive platform for ultralow-power electronics and spintronics [7–9]. Recently, the Kane-Mele model of the Honeycomb lattice was generalized to  $\alpha$ - $T_3$  lattice [10], where the tunable hopping parameter  $\alpha$  ( $0 \leq \alpha \leq 1$ ) interpolates between the honeycomb ( $\alpha = 0$ ) and Dice ( $\alpha = 1$ ) lattice [11–16] and was found to undergo a topological phase transition at  $\alpha = 1/2$  from QSHI with  $\sigma_{xy} = e^2/h$  ( $\alpha = 0$ ) to  $\sigma_{xy} = 2e^2/h$  ( $\alpha = 1$ ) [10]. The  $\alpha$ - $T_3$  lattice is characterized by a flat band along with two dispersive bands forming a Dirac cone similar to the Honeycomb lattice, hence realized as a pseudospin-1 Dirac-Weyl system [17]. Due to the spin-valley splitting of energy bands for  $0 < \alpha < 1$ , the system de-

picts a significantly rich phase diagram when a staggered magnetization term breaks the TRS of the QSH phase [10]. The property of the dispersionless zero-energy flat band and the variable berry phase [13] leads to many unconventional phenomena, such as unconventional Hall effect [13, 14, 18], higher Chern insulating phases [19–21], unconventional Anderson-localization [22], super-Klein-tunneling [23, 24], flat-band ferromagnetism [25], unusual Landau-Zener Bloch oscillations, and peculiar magnetic-optical effect [26]. The  $\alpha$ - $T_3$  lattice can naturally be built by growing a heterostructure of cubic Transition metal oxides ( $\text{SrTiO}_3/\text{SrIrO}_3/\text{SrTiO}_3$ ) or by creating an optical lattice with three pairs of counter-propagating laser beams [12]. It has been recently shown that  $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$  with critical doping can be mapped onto  $\alpha$ - $T_3$  lattice with  $\alpha = 1/\sqrt{3}$  [27]. Many other aspects of  $\alpha$ - $T_3$  lattice have been addressed so far, such as thermoelectric properties [28], optically irritated Floquet engineering [20, 29], Strain-induced pseudo magnetic field [30], and the effect of Rashba spin-orbit coupling [31, 32]. Although it is shown that extrinsic Rashba spin-orbit coupling (RSOC) is detrimental to the quantum spin Hall effect [6], it helps to realize the QAH effect. The QAH effect was predicted to be realized by introducing Rashba SOC and an exchange field in graphene [33–35] and was experimentally observed in magnetic insulators [3]. In the Dice lattice, introducing a RSOC in the presence of magnetic field [31] or Coulomb interaction [36], it is possible to get nearly flat bands with  $C = \pm 2$ . However, the fate of this quantum Hall phase in the presence of staggered potential or magnetization remains unexplored. In this paper, we aimed to study the possible topological phases in  $\alpha$ - $T_3$  lattice, mainly focusing on the Dice lattice, which is the  $\alpha = 1$  limit of general  $\alpha$ - $T_3$  lattice. The emergent topological phases arise due to the interplay of RSOC and ferromagnetic exchange coupling (EC) with staggered electric potential and magnetization terms individually. We carefully investigated the valley-polarized QAH (VPQAH)

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and argue that such staggered potentials are not always detrimental to the quantum Hall phases, comparing  $\alpha\text{-}\mathcal{T}_3$  lattice (pseudospin-1) with that of the Honeycomb lattice (pseudospin-1/2) with similar effects. Further, we present the anti-chiral edge states (ACES) associated with the topological metal (TM) phase of  $\alpha\text{-}\mathcal{T}_3$  lattice. Such ACES are recently been studied extensively in single-layer [16, 37] as well as composite forms of the modified Haldane model [38] and are experimentally evident [39]. The rest of the paper is arranged as follows.

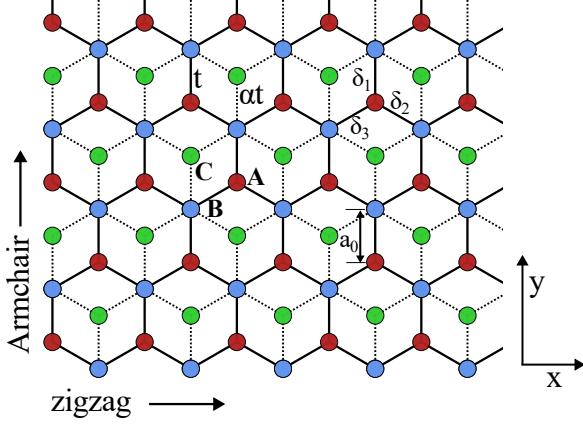


FIG. 1. Schematic of the  $\alpha\text{-}\mathcal{T}_3$  lattice with zigzag and armchair edges.  $\delta_n(n = 1, 2, 3)$  are three nearest neighbors drawn from the rim sublattice ( $A$  or  $C$ ).  $A, B$ , and  $C$  are denoted by the colors red, blue, and green respectively.

In Sec.II, we introduced the tight-binding model Hamiltonian for the  $\alpha\text{-}\mathcal{T}_3$  lattice with RSOC, exchange coupling, and external potentials. In Sec.III, we discussed the topological phase transitions with external potential and magnetization, which includes bulk band structure, topological invariant, Hall conductance, and edge modes of ribbon geometry and conclude in Sec.IV

## II. SYSTEM HAMILTONIAN AND FORMALISM

The  $\alpha\text{-}\mathcal{T}_3$  lattice with Hamiltonian with Rashba spin-orbit coupling and exchange term can be written as

$$H = H_0 + H_R + H_{ex} \quad (1)$$

where the first term

$$H_0 = -t \sum_{\langle i,j \rangle, s} C_{i,s}^\dagger C_{j,s} - \alpha t \sum_{\langle j,k \rangle, s} C_{j,s}^\dagger C_{k,s} + H.c. \quad (2)$$

describes the nearest neighbor (NN) hopping along directions  $\delta_1 = (0, a_0)$ ,  $\delta_2 = (-\frac{\sqrt{3}a_0}{2}, -\frac{a_0}{2})$ , and  $\delta_3 = (\frac{\sqrt{3}a_0}{2}, -\frac{a_0}{2})$ , from  $B$  and  $A(C)$  sites, with hopping strength  $t(at)$  with spin index  $s$ . Here,  $C_{i,s}^\dagger (C_{i,s})$  are electron creation (annihilation) operator with spin polarization  $s$  acting on site  $i$ .  $a_0$  is the distance between two sublattices. The second term

$$H_R = i\lambda_R \left[ \sum_{\langle i,j \rangle, s, s'} \hat{\mathbf{e}}_z \cdot (\boldsymbol{\sigma}_{s,s'} \times \mathbf{d}_{i,j}) C_{i,s}^\dagger C_{j,s'} + \alpha \sum_{\langle j,k \rangle, s, s'} \hat{\mathbf{e}}_z \cdot (\boldsymbol{\sigma}_{s,s'} \times \mathbf{d}_{j,k}) C_{j,s}^\dagger C_{k,s'} \right] + H.c. \quad (3)$$

describes the spin-mixing Rashba spin-orbit coupling with coupling strength  $\lambda_R(\alpha\lambda_R)$ , while  $\boldsymbol{\sigma}$  ( $\boldsymbol{\sigma}_x, \boldsymbol{\sigma}_y, \boldsymbol{\sigma}_z$ ) are Pauli matrices and  $\mathbf{d}_{ij}$  represents a unit vector pointing from site  $j(k)$  to site  $i(j)$  and finally the ferromagnetic exchange term modeled by

$$H_{ex} = \sum_{i,s} \boldsymbol{\sigma}_z \lambda_{ex} C_{i,s}^\dagger C_{i,s} + H.c. \quad (4)$$

Throughout this article, we measure the Rashba SOC and exchange energy in units of the hopping parameter  $t$ .

The momentum space Hamiltonian in the sublattice basis  $\{|A_\uparrow\rangle, |B_\uparrow\rangle, |C_\uparrow\rangle, |A_\downarrow\rangle, |B_\downarrow\rangle, |C_\downarrow\rangle\}^T$  obtained by Fourier transforming Eq.(1) can be described as,

$$H(k) = \begin{pmatrix} H_\uparrow & H_{\uparrow\downarrow} \\ H_{\downarrow\uparrow} & H_\downarrow \end{pmatrix} \quad (5)$$

where,  $H_\uparrow(H_\downarrow)$  is the spin-up (spin-down) Hamiltonian and  $H_{\uparrow\downarrow}(H_{\downarrow\uparrow})$  is the spin-mixing part of the Hamiltonian.

$$H_\uparrow(H_\downarrow) = \begin{pmatrix} +(-)\lambda_{ex} & f(k,t) & 0 \\ f^*(k,t) & +(-)\lambda_{ex} & f(k,\alpha t) \\ 0 & f^*(k,\alpha t) & +(-)\lambda_{ex} \end{pmatrix} \quad (6)$$

$$H_{\uparrow\downarrow} = \begin{pmatrix} 0 & \rho(k) & 0 \\ -\rho(-k) & 0 & -\alpha\rho(k) \\ 0 & \alpha\rho(-k) & 0 \end{pmatrix} \quad (7)$$

and,  $H_{\downarrow\uparrow} = H_{\uparrow\downarrow}^\dagger$  where,  $f(k,t') = f_x(k,t') - if_y(k,t')$ , and  $t'$  takes the values of either  $t$  or  $\alpha t$ .

$$f_x(k, t') = t' \left\{ \cos(a_0 k_y) + 2 \cos\left(\frac{\sqrt{3}a_0 k_x}{2}\right) \cos\left(\frac{a_0 k_y}{2}\right) \right\},$$

$$f_y(k, t') = t' \left\{ \sin(a_0 k_y) - 2 \cos\left(\frac{\sqrt{3}a_0 k_x}{2}\right) \sin\left(\frac{a_0 k_y}{2}\right) \right\},$$

$$\rho(k) = i\lambda_R \left\{ e^{-ia_0 k_y} + 2 e^{\frac{ia_0 k_y}{2}} \cos\left(\frac{\sqrt{3}a_0 k_x}{2} + \frac{2\pi}{3}\right) \right\}$$

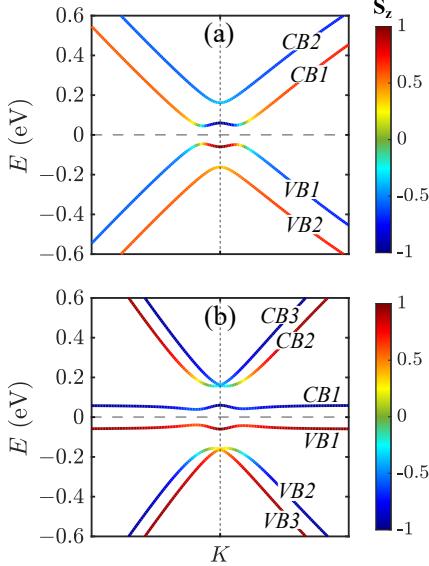


FIG. 2. Band structure of the honeycomb lattice ( $\alpha = 0$ ) [upper panel] and dice lattice ( $\alpha = 1$ ) [lower panel] for  $\lambda_R \neq 0$ ,  $\lambda_{ex} \neq 0$ . The band color depicts the  $z$ -component of the spin texture. The tight binding parameters used in the unit of  $t$  are  $\lambda_R = 0.05$ ,  $\lambda_{ex} = 0.06$ .

$$\rho(-k) = i\lambda_R \left\{ e^{ia_0 k_y} + 2 e^{-\frac{ia_0 k_y}{2}} \cos \left( \frac{\sqrt{3}a_0 k_x}{2} - \frac{2\pi}{3} \right) \right\}$$

The topological invariant associated with the system is calculated using berry curvature for individual bands in the  $k_x - k_y$  plane [40]. The  $z$ -component of the berry curvature was calculated numerically using [40]

$$\Omega_n(k_x, k_y) = -2 \sum_{n' \neq n} \text{Im} \left[ \frac{\langle u_n | \frac{\partial H}{\partial k_x} | u_{n'} \rangle \langle u_{n'} | \frac{\partial H}{\partial k_y} | u_n \rangle}{(E_{n'} - E_n)^2} \right] \quad (8)$$

for  $n$ th band for each  $k$ -points, summing over all other bands  $n'$ .  $|u_n\rangle$  and  $E_n$  are block states and eigenvalues of the Hamiltonian given in Eq.(1) for the  $n$ th band. The surface integral of the Berry curvature  $\Omega_n$  over the first Brillouin zone gives  $2\pi C_n$ , where  $C_n$  is called the Chern number or TKNN index [41, 42] of  $n$ th band, which is the topological invariant of the system.

### III. RESULTS AND DISCUSSION

#### A. Momentum interlocked spin polarization of bands

The bulk band structure of  $\alpha$ - $T_3$  lattice with Rashba SOC and exchange coupling can be obtained by diagonalizing  $6 \times 6$  spin-full Hamiltonian of Eq.(5) for each

crystal momentum. In the absence of spin-orbit coupling and exchange term, ( $\lambda_R = 0$ ,  $\lambda_{ex} = 0$ ), due to spin degeneracy, the bands are four-fold for  $\alpha = 0$  and six-fold for  $\alpha = 1$  degenerate respectively near the Dirac points. The inclusion of Rashba SOC term, ( $\lambda_R \neq 0$ ,  $\Lambda_{ex} = 0$ ) couples the electron's spin to its momentum in the plane and breaks the inversion symmetry in the case of  $\alpha = 0$ , leading to the splitting of the bands into four non-degenerate bands by an amount proportional to Rashba coupling strength  $\lambda_R$  [5, 43, 44]. In the case of  $\alpha = 1$ , though a spin-momentum coupling arises due to Rashba SOC, however, the inversion symmetry is still preserved [45], and this allows the three spin-degenerate bands to remain degenerate with their corresponding spin-flipped counterparts. The exchange field alone ( $\lambda_R = 0$ ,  $\Lambda_{ex} \neq 0$ ) makes the bands fully spin-polarized. The spin-up (spin-down) bands are pushed upward (downward) by an amount of exchange field, and the time-reversal symmetry (TRS) is broken due to the spin polarization. The simultaneous presence of RSOC and exchange field ( $\lambda_R \neq 0$ ,  $\Lambda_{ex} \neq 0$ ) makes the bands nondegenerate, and a bulk gap opens up near the Dirac points. In Fig. 2, we presented the bulk energy spectrum at  $K$  - valley for two limiting cases,  $\alpha = 0$ , which is Honeycomb lattice (pseudospin- $\frac{1}{2}$ ) in the upper panel and  $\alpha = 1$ , which is the Dice lattice (pseudospin-1) in the lower panel. The expectation value of the  $z$ -component of the spin is shown as the band color. Our results for  $\alpha = 0$  are consistent with earlier studies [33]. Due to the interplay of RSOC and EC, a momentum-dependent spin texture is observed near the band-crossing points. The bulk gaps obtained in both Honeycomb and Dice lattice 2 are found to be topological in nature with a total Chern number  $|C| = 2$  and exhibit a QAH phase with  $\sigma_{xy} = 2e^2/h$  [31, 33]. Although the  $\alpha$  plays an important role in tuning the spin Hall phase in the case of ISOC [10], it does not change the QAH phase obtained by RSOC and EC. The impact of  $\alpha$  on the spectral properties, along with different RSOC and EC strengths, are shown in Appendix A. However, the bulk gaps are sensitive to external staggered fields that can even modify their existing QAH phases, as we will see in the later sections.

#### B. Staggered electric field induced valley polarized quantum anomalous Hall

In this section, we investigate the effect of a staggered electric potential on the Rashba SOC and exchange field induced dice lattice and compare the results with that of the honeycomb lattice. Here, for the Dice lattice, we consider a staggered electric potential  $\Delta$ , i.e., the electric potential on A and C sublattices are opposite but zero in the B sites. Therefore, we add another term  $H_\Delta = \sum_{i,s} \Delta_i C_{i,s}^\dagger C_{i,s}$  in the Hamiltonian of Eq.(1), which in

sublattice basis reads as,

$$H_\Delta = \Delta \sigma_0 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

For the Honeycomb lattice, such a staggered potential is conventionally realized taking  $+\Delta$  on  $A$ - and  $-\Delta$  on  $B$ -sublattices. The staggered electric potential ( $\Delta$ ) breaks the inversion symmetry, the bands are no longer symmetric under the valley exchange. In Fig.3 (a1)-(a3) and (b1)-(b3) shows the bulk band structure near the two inequivalent valleys for the Honeycomb [left panel] and Dice lattice [right panel] respectively. From the plots, we found that the energies of the bands exactly at  $K$  and  $K'$  for Honeycomb lattice are  $E_{2,3} = \pm(\Delta + \eta\lambda_{ex})$  and  $E_{1,4} = \pm\sqrt{(\Delta - \eta\lambda_{ex})^2 + 9\lambda_r^2}$  and for Dice lattice are  $E_{3,4} = \pm(\Delta + \eta\lambda_{ex})$ ,  $E_{1,2,5,6} = \frac{1}{2}(\pm\Delta \pm \sqrt{(\Delta - 2\eta\lambda_{ex})^2 + 36\lambda_r^2})$  with  $\eta = \pm 1$  representing the  $K$  and  $K'$  respectively. For the variable,  $\Delta$ , the bulk gap  $2(\Delta + \eta\lambda_{ex})$  first closes at  $\Delta = \lambda_{ex}$  and then opens again for  $\Delta > \lambda_{ex}$  at  $K'$  ( $\eta = -1$ ), whereas, at  $K$ , the bulk gap keep increases with  $\Delta$  in both  $\alpha = 0$  & 1 cases. The bulk bands near both the valleys for three different values of staggered potential before band crossing ( $\Delta = 0.02t$ ), at the critical point ( $\Delta = 0.06t$ ) and after the band crossing ( $\Delta = 0.1t$ ) in both  $\alpha = 0$  & 1 cases shown in Fig. 3. The band color represents the  $z$ -component of berry curvature, where the change in polarity of berry curvature at the band crossings suggests a topological phase transition for individual bands. The plot of bulk bandgap ( $\Delta E_{direct}$ ) and total chern number ( $C$ ) of occupied bands as a function of potential strength  $\Delta$  are shown in Figs.3(c) and 3(d). Although Fig.3 shows multiple band crossings among the higher energy bands away from the Fermi energy, the total Chern number below the Fermi energy remains the same and only the bulk gap closing and opening modifies the topological phase of the system very similar to a hidden topological phase transition shown recently in Honeycomb lattice [38]. The band crossing at the bulk gap modifies the topology of the two systems differently. For the Honeycomb lattice, the topological phase goes from a higher Chern insulator (HCI) with  $|C| = 2$  to a bulk insulator phase with  $|C| = 0$  as shown by the blue curve in Fig.3(c). Whereas for dice lattice, the phase goes from HCI ( $|C| = 2$ ) to another Chern insulating phase with  $|C| = -1$  as shown by the blue curve in Fig.3(d). The negative sign implies a switch in the chirality of the edge modes associated with the Hall phase, which we have verified by numerically calculating the edge bands in Sec.III D. So, by applying an external staggered electric potential of strength equal to the exchange coupling, one can switch the chirality of topologically protected edge states in a pseudospin-1 system, like a dice lattice. Changing the sign of the electric potential can reverse the valley polarization and chirality of the edge states.

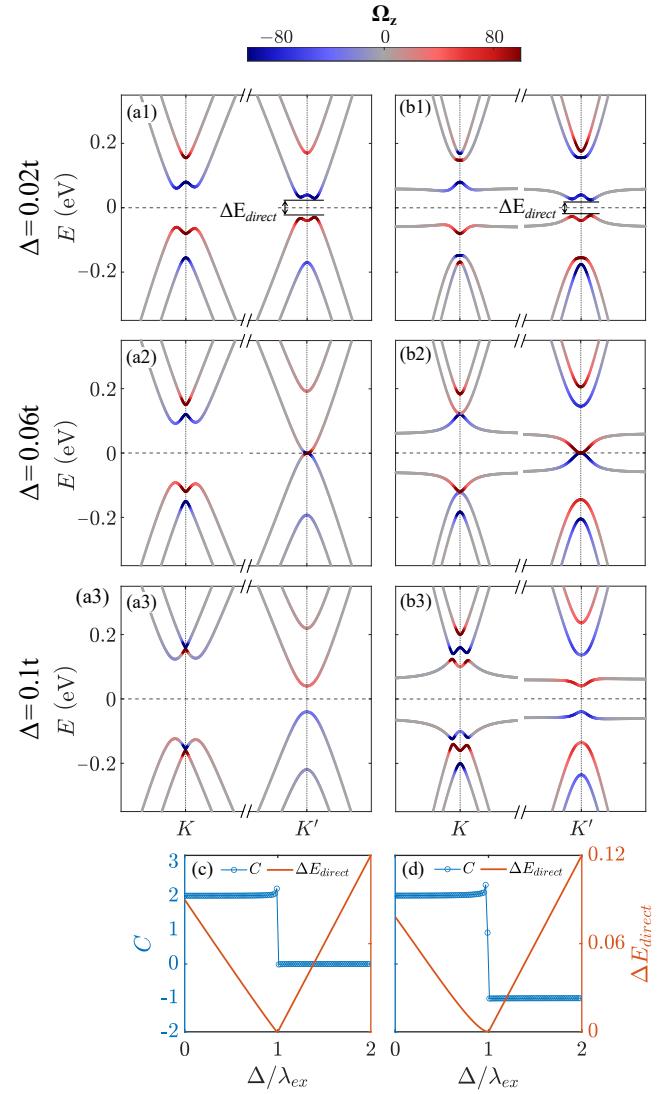


FIG. 3. Band structures of the gapped phase in the presence of RSOC and exchange coupling are shown for different values of  $\Delta$  near the two Dirac points  $K$  and  $K'$  for ( $\alpha = 0$ ) honeycomb lattice [(a1)-(a3) of left panel] and ( $\alpha = 1$ ) Dice lattice [(b1)-(b3) of right panel]. Band color represents the  $z$  component of the berry curvature. The total Chern number of all occupied bands and the bulk band gap as a function of staggered potential for Honeycomb lattice (c) and Dice lattice (d). The parameters used are the same as that of Fig.2

### C. Staggered magnetization induced topological metal (TM) phase

Here, we discuss the effect of a staggered magnetization along with the RSOC and EC. We consider an  $A-C$  sublattice staggered magnetization [10]  $M$  by adding a term  $H_M = \sum_{i,s} \sigma_z M_i C_{i,s}^\dagger C_{i,s}$  to the original Hamiltonian.

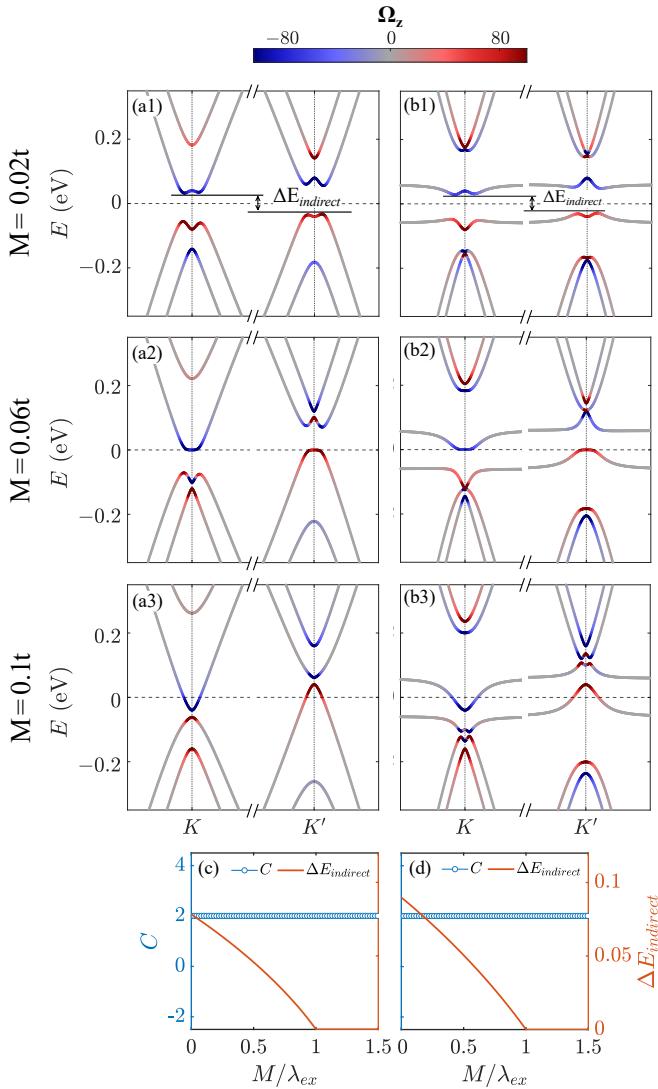


FIG. 4. Band structures of the gapped phase in the presence of RSOC and exchange term are shown near the two Dirac points  $K$  and  $K'$  for different values of staggered magnetization  $\Delta M$  for honeycomb lattice [(a1)-(a3) of left panel] and ( $\alpha = 1$ ) Dice lattice [(b1)-(b3) of right panel]. Band color represents the  $z$  component of the berry curvature. The total Chern number ( $C$ ) of all occupied bands and the bulk band gap as a function of staggered potential for Honeycomb lattice (c) and Dice lattice (d). The parameters used are the same as that of Fig.2

nian Eq.(1), which in sublattice basis reads as,

$$H_M = M\sigma_z \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

For the Honeycomb lattice such a staggered magnetization is implemented with an additional  $M\sigma_z\tau_z$  term to the Hamiltonian [46]. The initial gapped systems ( $M = 0$ ) lack TRS, and now introducing the staggered  $M$  term breaks the particle-hole symmetry. How-

ever, the overall system preserves chiral symmetry, which is a combined symmetry of time-reversal and particle-hole symmetries. Hence, the energy dispersion obeys  $E(-k) = -E(k)$ . The band energies exactly at  $K$  and  $K'$  for Honeycomb lattice are  $E_{2,3} = \eta(\Delta \pm \lambda_{ex})$  and  $E_{1,4} = -\eta M \pm \sqrt{\lambda_{ex}^2 + 9\lambda_r^2}$  and for Dice lattice are  $E_{3,4} = \eta(M \pm \lambda_{ex})$ ,  $E_{1,2,5,6} = \frac{1}{2}(-\eta M \pm \sqrt{(M \pm 2\lambda_{ex})^2 + 36\lambda_r^2})$  with  $\eta = \pm 1$  representing the  $K$  and  $K'$  respectively. Fig.4(a1) - 4(a3) and 4(b1) - 4(b3) shows the bulk band structure near the two inequivalent Dirac points of Honeycomb lattice [left panel] and dice lattice [right panel] under the influence of three different magnetization strengths  $M = 0.02t (< \lambda_{ex})$ ,  $M = 0.06t (= \lambda_{ex})$ , and  $M = 0.1t (> \lambda_{ex})$  respectively. The color of the bands indicates the berry curvature polarization and distribution along the  $k$ -path. The bulk bandgap and the total Chern number are plotted with magnetization strength  $M$  in Fig.4(c) and 4(d). As the magnetization strength increases, the conduction band at the  $K$  point and the valence band at the  $K'$  point come closer and touch the Fermi energy at  $M = \lambda_{ex}$  (4(a2) and 4(b2)) leading to the the bulk indirect band gap  $\Delta E_{indirect} = 2(M - \lambda_{ex})$  to be vanished (solid red curve), and the system becomes metallic. As the bands are associated with non-zero Chern numbers and no band crossing between the valence and conduction bands are observed, we anticipate this new metallic phase to be a topological metal (TM), conducting phase hosting the co-existence of in-gap bulk states with edge states. Later in Sec.III D, we discussed the nanoribbon band structures and confirmed that the system experiences a phase transition from HCl ( $C = 2$ ) to a TM at  $M = \lambda_{ex}$ . A similar phase transition has previously been observed in  $\alpha$ - $T_3$  lattice at  $\alpha = 1/2$  for a Modified Haldane model [16]. We found that the staggered magnetization term is detrimental to the QAH phase for both Honeycomb and Dice lattice, however, it opens up a new platform to study unconventional edge band structures.

#### D. Chiral and Half antichiral edge states

The concept of bulk-boundary correspondence states that topological phases possess localized edge states protected by nontrivial bulk topological invariants. The edge states in quantum anomalous Hall materials are generally associated with the total Chern number of the valence bands. Here we have discussed the edge states of the zigzag nanoribbon (ZNR) structure that explain the VPQAH phase and the TM phase individually obtained by two different staggered terms in the Hamiltonian, as discussed earlier in Sections III B and III C.

We constructed the honeycomb and dice lattice nanoribbon geometries by considering periodic boundary conditions along the direction of the zigzag edge and open boundary conditions along the perpendicular direction. We then obtained the band structure of each geometry to visualize the edge states (see Fig.1). For the

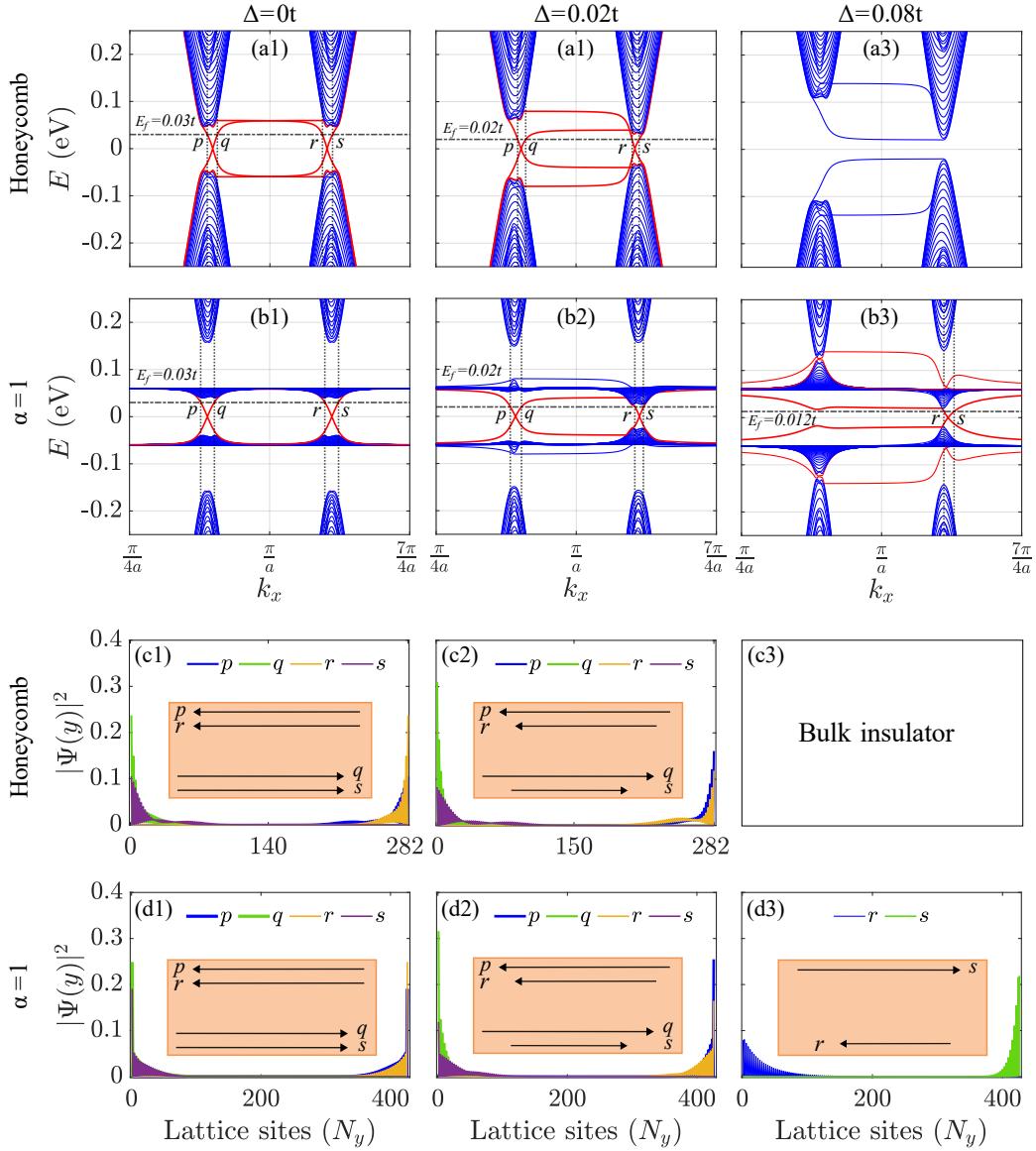


FIG. 5. (upper panel) The band structures of zigzag nanoribbon with applied Rashba spin-orbit coupling and exchange term for Honeycomb lattice [(a1) – (a3)] and dice lattice [(b1) – (b3)] for three different values of staggered electric potential  $\Delta$ , where red and blue color indicates the conducting edge bands and bulk bands respectively. The zigzag chain contains  $N_y = 282$  AB sites for the Honeycomb lattice and  $N_y = 426$  ABC sites for the dice lattice. (lower panel) probability density distribution with the lattice sites along the finite direction corresponding to the edge modes shown in the upper panel, where the inset shows the localization and chirality of the modes along a rectangular slab. Parameter used are same as Fig.2

honeycomb lattice, the ZNR contains sublattices A and B along opposite edges, whereas, for the Dice lattice, we have considered a C-A edged ribbon, i.e., where the top edge has A sublattices and the bottom edge contains C [47, 48]. Figs.5(a1) – 5(a3) and Figs.5(b1) – 5(b3) shows the ribbon band structure for different staggered electric potentials for honeycomb and Dice lattice, respectively with the Fermi energy crossings of the edge bands. The red and blue color denotes conducting edge bands and gapped bulk bands. The probability density distribution with the lattice sites along the perpendicular direction corresponding to edge modes for a given Fermi energy

are shown in Figs.5(c1) – 5(c3) and Figs.5(d1) – 5(d3) where the insets suggest the localization and chirality of the edge modes in rectangular slab. Figs.5(a1) and 5(b1) refer to edge bandstructure corresponding to bulk band shown in Figs.2(d) and 2(h) where no external potential is applied. Two pairs of counter-propagating chiral edge modes are consistent with the total Chern number  $C = 2$  below the given Fermi energy  $E_f = 0.03t$ . For a finite value of staggered electric potential ( $\Delta = 0.02t$ ) below the critical point, those two pairs of chiral edge states persist, however one pair of edge modes spread into the bulk and has a larger localization length due to

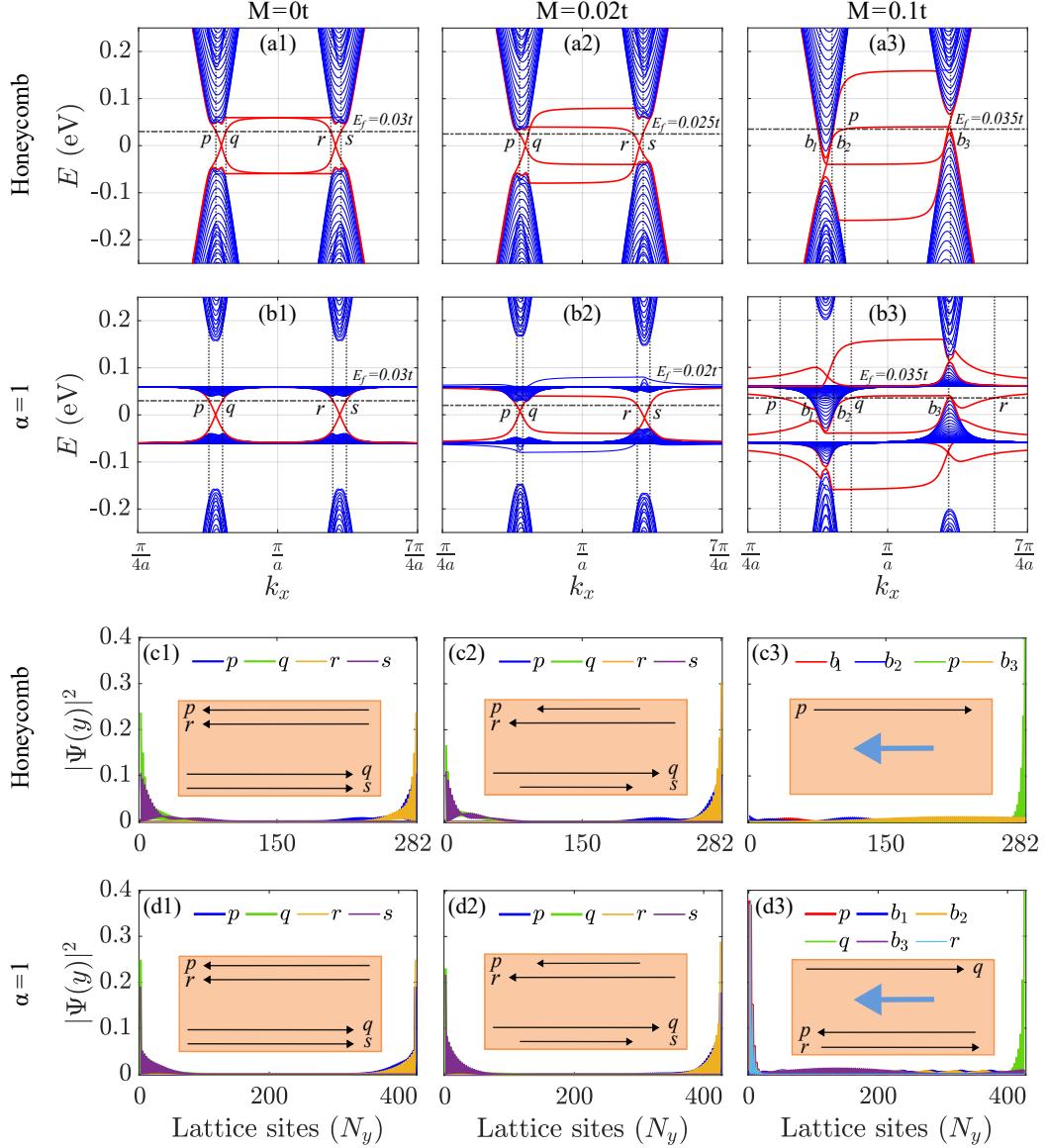


FIG. 6. (upper panel) The band structures of zigzag nanoribbon with applied Rashba spin-orbit coupling and exchange term for Honeycomb lattice [(a1)–(a3)] and dice lattice [(b1)–(b3)] for three different values of staggered magnetization  $\Delta M$ , where red and blue color indicates the conducting edge bands and bulk bands respectively. The zigzag chain contains  $N = 282$  AB sites for the Honeycomb lattice and  $N = 426$  ABC sites for the dice lattice. (lower panel) probability density distribution with the lattice sites along the finite direction corresponding to the edge modes shown in the upper panel, where the inset shows the localization and chirality of the modes along a rectangular slab. Parameter used are same as Fig.2

a smaller bulk gap of one valley compared to the other valley [Figs.5(a2), 5(b2) and Figs.5(c2), 5(d2)]. The wave function of an edge state typically decays as  $e^{-y/\xi} \cos kx$ , where  $y$  is the distance from the edge, wave vector along the edge, and  $\xi$  is the localization length, which determines how fast the wave function decays into the bulk, and is inversely proportional to the band gap.

After the critical point, there are no edge modes conducting from the valence band to the conduction band for honeycomb lattice [Fig.5(a3)], hence turning into a bulk insulator. However, in the case of the dice lattice, now there is one pair of edge modes in each edge prop-

agating in opposite directions [Fig.5(b3)]. Notably, the contribution to the conducting edge modes comes from a specific valley, and their chirality is now altered. This valley-specific behavior gives rise to a valley-polarized QAH phase with a change in sign. In such a gapped system, the Fermi energy is chosen in the bulk gap that crosses only the conducting edge modes, which appears in a quasi-1D ribbon geometry. Therefore, the total Chern number of the bands below the Fermi energy includes all valance bands, and it corresponds to the total number of edge modes [Figs.3(c) and 3(d)].

In the case of applied staggered magnetization, the

system remains bulk-gapped as long as  $M < \lambda_{ex}$  and the quantized number of edge modes propagate along the edges in opposite directions protected by the total Chern number  $C = 2$  as shown in Figs.6(a2), 6(b2), 6(c2) and 6(d2). The bulk gap vanishes for  $M > \lambda_{ex}$ , and hence, the total Chern number of the valence bands does not correspond to the edge modes directly. For Fermi energy close to charge neutrality, there exist edge modes(red) [ $p$  in Fig.6(a3) and  $p, q$  and  $r$  in Fig.6(b3)] propagating along the edges with a smaller localization length [Fig.6(c3) and Fig.6(d3)] along with conducting bulk modes (blue) [ $b_1, b_2$  and  $b_3$  in Fig.6(a3) and 6(b3)]. The coexistence of edge modes and in-gap bulk modes are found recently in the modified Haldane model for both Honeycomb lattices [37, 49–51] and  $\alpha$ - $T_3$  lattice [16, 29] where co-propagating edge modes exist in the two opposite edges along with modes propagating in the bulk in opposite direction. This pair of co-propagating edge modes is known as anti-chiral edge states and are found in a topological metal phase of matter, which has also been recently experimentally realized [39, 52]. In our case, the Honeycomb lattice host one unpaired edge mode  $p$  propagating only on one edge of the ribbon [Fig.6(c3)] and compensated by the counter-propagating bulk. Whereas, for the dice lattice edge modes  $p$  and  $r$  being on the same edge and counter-propagating, cancels each other, resulting into a single edge mode  $q$  propagating on the other edge, which make it equivalent to the honeycomb case. These unpaired edge states, referred to as half-antichiral edge states (HACES), were recently proposed in a composite Haldane-modified Haldane bilayer system of Honeycomb lattice [38].

### E. Anomalous Hall conductance

In this section, we calculate the anomalous Hall conductivity for the Honeycomb and Dice lattice with RSOC and EC, with two individual staggered terms as described in Secs.III B and III C. We computed the Hall conductivity by numerically integrating the Berry curvature (BC) of all occupied electronic states over the entire Brillouin zone (BZ). This involves summing up all the filled bands in the system [40].

$$\sigma_{xy} = \frac{\sigma_0}{2\pi} \sum_n \int \Omega_n(k_x, k_y) f(E_{k_x, k_y}^n) dk_x dk_y \quad (9)$$

Where  $\Omega_n$  is the berry curvature for  $n^{th}$  band from Eq.(8),  $f(E) = 1/[1 + e^{(E-E_f)/K_B T}]$  is the Fermi-Dirac distribution function where  $E_f$  and  $T$  signifies Fermi energy and absolute temperature respectively,  $E_{k_x, k_y}^n$  is the energy eigenvalues for  $n^{th}$  band and  $\sigma_0 = e^2/h$ . When the Fermi energy lies in a band gap, the Fermi-Dirac distribution function  $f(E)$  at zero absolute temperature equals unity, and the total contribution of all occupied states comes from bands below the Fermi energy. Then, the integration over the BZ gives the total Chern num-

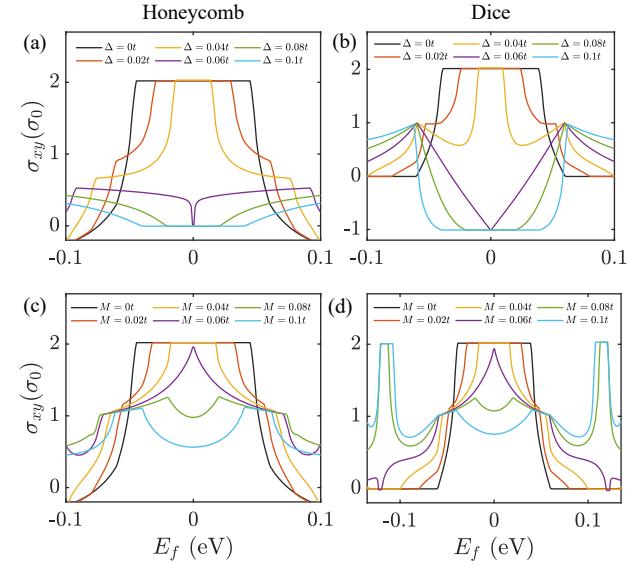


FIG. 7. QAHC for different values of [upper panel] staggered electric potential  $\Delta$  for Honeycomb lattice (a) and Dice lattice (b) and [lower panel] staggered magnetization  $M$  for Honeycomb lattice (c) and Dice lattice (d) as a function of Fermi energy.

ber of the bands below the Fermi energy, and we get a plateau  $\sigma_{xy} = |C_n|e^2/h$ .

The conductivity decays when the Fermi energy lies outside the bulk gap or when the gap closes. Fig.7(a) and 7(c) shows the anomalous Hall conductivity for the Honeycomb lattice and Dice lattice as a function of Fermi energy ( $E_f$ ) in the unit of  $\sigma_0$  for different values of staggered electric potential  $\Delta$ . The width of the Hall plateau decreases with the gap ( $\Delta E_{direct}$ ), and the plateau completely diminishes when the gap is zero at  $\Delta = \lambda_{ex}$ . As the gap reopens at  $K'$  a new quantized plateau arises, suggesting a QAH phase transition. The Hall plateau changes from  $2e^2/h$  (QAH phase) to 0 (BI phase) for the honeycomb lattice and from  $2e^2/h$  (QAH phase) to  $-e^2/h$  (VPQAH phase), where the negative sign refers to a change in the chirality of the edge modes. Fig.7(c) and 7(d) show the QAHC as a function of Fermi energy for different values of staggered magnetization  $M$ . In this case, the indirect bulk band gap  $\Delta E_{indirect}$  decreases with increasing  $M$  and vanishes at  $M = \lambda_{ex}$  and so the QAH plateau. For  $M > \lambda_{ex}$ , the system remains metallic, and the Hall conductivity is no longer quantized. In the TM phase, the non-zero contribution to the QAHC for Fermi energy close to the charge neutrality arises from the half anti-chiral edge states described previously. Fig.7(d) shows two more smaller plateau regions for Fermi energy away from charge neutrality. Those two plateaus change from 0 to  $2e^2/h$  at the band crossing between VB1 and VB2 at valley- $K$  and between CB1 and CB2 at valley- $K'$ . When Fermi energy lies in the region of a small gap between VB2 and VB3, the AHC is solely contributed by VB1 and VB2, resulting in

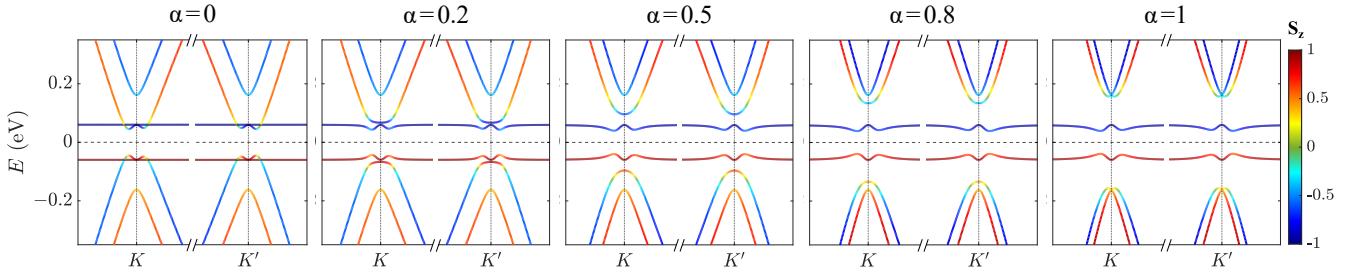


FIG. 8. Band structure obtained from  $H$  in Eq.(1) near the two inequivalent  $K$ -points for different values of  $\alpha$ , for hamiltonian parameters used in terms of  $t$  are,  $\lambda_R = 0.05$ ,  $\lambda_{ex} = 0.06$ . The color of the bands represents expectation value of the z-component of the spin.

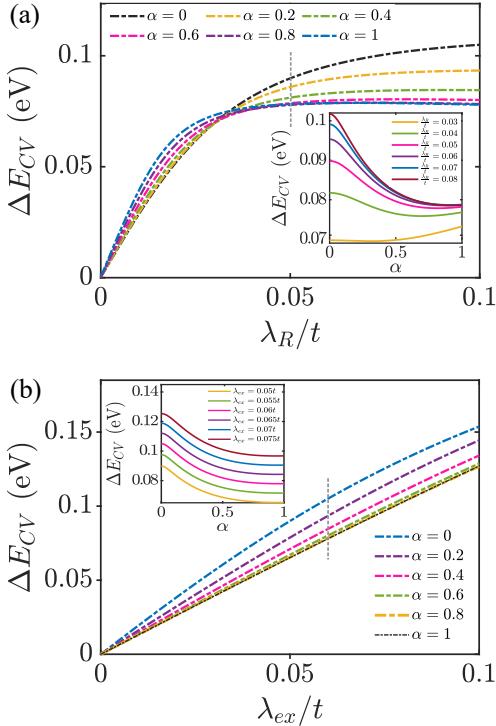


FIG. 9. Band gap vs (a) Rshba SOC strength and (b) exchange coupling for different values of  $\alpha$ . The fixed parameters are kept the same as in Fig.2.

#### IV. CONCLUSION

We have investigated the electronic band structures and topological properties of a gapped phase obtained by the interaction of Rashba SOC and exchange coupling for a pseudospin-1 system,  $\alpha$ - $T_3$  lattice with  $\alpha = 1$  and compared the results with that of a pseudospin-1/2 system, Honeycomb lattice. We also uncover the effect of external staggered electric potential and magnetization on these topological phases individually. We observed a topological phase transition from the QAH phase ( $2e^2/h$ ) to a bulk insulator for Honeycomb ( $\alpha = 0$ ) and to a valley-polarized QAH phase ( $-e^2/h$ ) with a flip in chirality/edge for Dice lattice ( $\alpha = 1$ ) at a staggered electric potential equal to the exchange coupling. For an applied staggered magnetization, the Chern number is insufficient to characterize the topological phase of the system as it experiences a phase transition from QAH ( $2e^2/h$ ) phase to a TM phase at  $M = \lambda_{ex}$ . The TM phases in both Honeycomb and Dice lattice host single edge mode along one edge, referred to as half-antichiral edge state, along with counter-propagating bulk modes. In the TM phase, the bulk gap closes, the system becomes metallic, and QAH is no longer quantized. However, contrary to the honeycomb lattice, for Fermi energy away from the bulk gap, a pair of new quantized plateaus ( $2e^2/h$ ) arises for the dice lattice.

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$\sigma_{xy} = 0$  and  $\sigma_{xy} = |2|e^2/h$  respectively before and after the band crossing (Fig.7(d)), as the total Chern number  $C = 2$  is the sum of the two Chern numbers of VB2 and VB3. Similarly, we observe another plateau region for the energy gap between CB1 and CB2 as the Chern number of CB1 and VB1 are equal and opposite signs, they cancel out, resulting in the total Chern number being the same as that in the valance band gap.

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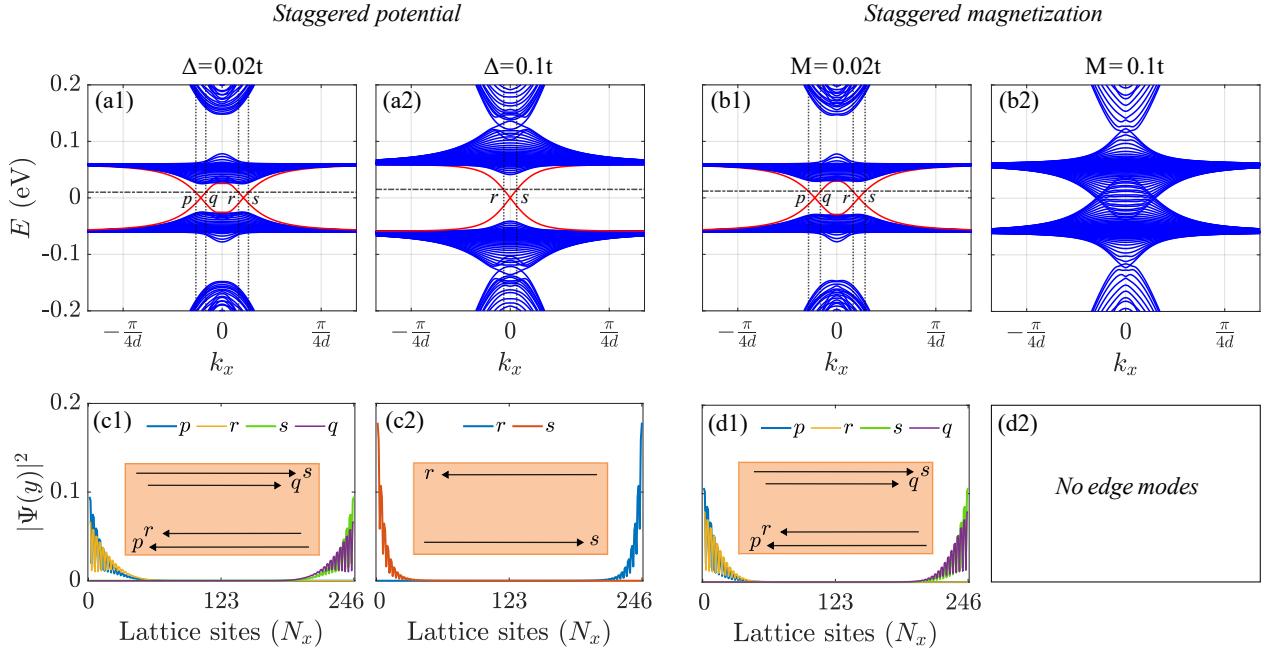


FIG. 10. (upper panel) The band structure of Dice lattice armchair nanoribbon for staggered potential  $\Delta < \lambda_{ex}$  (a1) and  $\Delta > \lambda_{ex}$  (a2) and, staggered magnetization  $M < \lambda_{ex}$  (b1) and  $M > \lambda_{ex}$  (b2). (lower panel) The probability densities along the width corresponding to edge modes in the upper panel. The width of the nanoribbon is taken as  $123\sqrt{3}a_0$  along the  $x$ -direction. Other parameters used are same as that of Fig.2

### Appendix A: Beyond Dice lattice : $0 < \alpha < 1$

In this manuscript, so far we have discussed the QAH phase induced by RSOC and exchange coupling on dice lattice, i.e.,  $\alpha = 1$  case of the model discussed in sec.II. The parameter hopping  $\alpha$  in  $\alpha$ - $\mathcal{T}_3$  lattice is known to tune the topology of the system with Haldane and modified Haldane model [16], intrinsic SOC [10], or Floquet engineering [29]. However, we observed that the topological phase obtained by RSOC and exchange term remain unchanged irrespective of  $\alpha$  values. Fig.8 shows the band structures of the gapped phase ( $\lambda_R \neq 0$ ,  $\lambda_{ex} \neq 0$ ) obtained from Eq.(1) for intermediate values of alpha including two limiting values  $\alpha = 0$  (honeycomb lattice) and  $\alpha = 1$  (dice lattice), where the dashed line indicates the Fermi energy and the color of the bands represents the expectation values of the z-component of spin. At  $\alpha = 0$ , the  $6 \times 6$  spinful Hamiltonian mimics the  $4 \times 4$  Hamiltonian of a Honeycomb lattice, apart from the two completely flat bands separated by  $2\lambda_{ex}$  arising from the onsite exchange coupling term of the isolated  $C$  sublattice. These two bands, being completely nondispersive, do not contribute to the berry curvature and conductivity of the system. For finite nonzero value of  $\alpha$ , the middle bands become dispersive; however, the bulk gap remains open for any  $\alpha$ . Therefore, although the band gap varies, no new topological phase arises. The variation in the band gap  $\Delta E_{CV}$  with Rashba SOC strength and exchange coupling for different  $\alpha$  are shown in Figs.9

(a) and 9 (b), where the insets show the band gap plot with alpha for different RSOC and exchange coupling, respectively. For any specific  $\alpha$ , the band gap opens when both  $\lambda_R$  or  $\lambda_{ex}$  is non-zero. For lower (higher) values of Rashba coupling, the band gap increases (decreases) with  $\alpha$ . However, it always increases with the exchange coupling. The gray lines in the band gap plots indicate the parameters and the gap corresponding to different  $\alpha$  for the band structure shown in Fig.8.

### Appendix B: Armchair edge bands

To obtain the band structure of the armchair nanoribbon, the periodic boundary condition along the  $y$ -axis (armchair edge) and open boundary condition along the  $x$ -direction (zigzag edge) are considered (see Fig.1). The upper panel of Fig.10 shows the band structure of armchair nanoribbons of dice lattice ( $\alpha = 1$ ) and the Fermi energy crossings of the edge bands, and the lower panel shows the probability density distribution across the lattice sites along the direction of finite width, with inset showing schematic of chirality of edge modes in a rectangular slab. For the staggered potential, the Fermi energy crosses two (one) pair of edge bands before (after)  $\Delta = \lambda_{ex}$ , consistent with the HCI (CI) phase [Figs.10(a1) and 10(a2)]. It is also important to note that the reversal of the chirality of edge modes after  $\Delta = \lambda_{ex}$  is also consistent with that of the zigzag edge and flip in the sign

of QAH. However, since the armchair geometry overlaps the two valleys, the valley polarization is not evident in contrary to the zigzag edge. For the staggered magnetization, before  $M = \lambda_{ex}$ , the Fermi energy crosses two pairs of edge bands and hence is a HCl phase; however, for  $M > \lambda_{ex}$  the conduction bulk states overlap with the valance band bulk states and no edge bands are ob-

served thus appearing as a trivial metal [Figs.10(b1) and 10(b2)], in contrary to the zigzag edge bands. This is because the edge bands for TM phase in Fig.6 (b3) connecting the valance band of  $K$ -valley to the conduction band of  $K'$ -valley and shielded from the view by the in gap bulk bands as soon as the indirect band gap is closed. Hence, valley separation is crucial to visualize these half anti-chiral edge states.

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