Flat Bands and Edge Currents in Dice-Lattice Ladders

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We introduce the concept of “dice ladders”. These are ribbons of the dice two-dimensional lattice previously studied in F. Wang and Y. Ran, Phys. Rev. B 84, 241103 (2011), that display nontrivial topological properties, such as Chern numbers equal to 2. By studying the dice-lattice tight-binding model in the presence of Rashba spin-orbit coupling and an external magnetic field, we observed that dice ladders qualitatively display similar properties to their two-dimensional counterpart. This includes flat bands near the Fermi level, edge currents and edge charge localization near zero energy when open boundary conditions are used, two chiral edge modes, and a nonzero Hall conductance. While the finite number of momenta in the short direction when using cylindrical or toroidal boundary conditions prevents having sharp integer Chern numbers, the dice ladders provide useful toy models that qualitatively resemble the true topological planar systems. Using ladders has the important advantage that correlation effects, such as Hubbard $U$ couplings, can be studied with powerful computational many-body techniques specialized to one-dimensional geometries. Our results thus pave the way towards numerical studies of the combined influence of flat bands, edge currents, and Hubbard correlation in a single model, one of the frontiers in theory of Quantum Materials.

I. INTRODUCTION AND DICE LATTICE

In his early seminal paper, Haldane proposed a tight-binding model on a honeycomb lattice, including a staggered flux pattern, that displays the integer quantum Hall effect [1]. Time reversal symmetry is broken by the complex-valued second-neighbor hoppings and no external magnetic fields are needed. Generalizations led to the widely addressed concept of topological insulators [2–4]. Years later, it was also discovered that a similar approach works even for the fractional quantum Hall effect, also without employing Landau levels and large magnetic fields [5–9]. The essence is to search for models that display quasi two-dimensional flat bands with a nonzero Chern number, which arises from the integral of the Berry phase over the two-dimensional Brillouin zone. These bands must be isolated from other bands to resemble Landau levels. The topological band structures created by this procedure are of considerable current interest. This type of models are referred to as lattice Chern insulators. The Chern number equals the number of chiral edge modes.

In particular, the two-dimensional Haldane model that uses two triangular lattices was generalized to three by Wang and Ran [10]. By this procedure fine tuning of parameters is avoided, and the honeycomb lattice becomes the dice lattice [11–13], illustrated in Fig. 1, via the addition of an extra site at the center of each hexagon. This bipartite lattice has two types of sites: two thirds with coordination three and one third with coordination six. The unit cell contains three sites, thus leading to three bands. What is remarkable is that this model at the non-interacting tight-binding level and with a small Zeeman field—with hoppings only between nearest-neighbor sites and with the inclusion of Rashba spin-orbit coupling—display bands with Chern number $C$ equal to $\pm 2$ [14], as opposed to the still non-trivial but more standard $C = 1$ of the Landau levels in the integer quantum Hall effect.

The dice lattice is not merely an abstract geometry but it can be realized via a trilayer superlattice grown in the [111] direction [15], such as in SrTiO$_3$/SrIrO$_3$/SrTiO$_3$. From the theory perspective, the $\alpha$-$T_3$ model, which interpolates between the honeycomb and the dice lattices, has also received considerable attention [16–19]. In dice lattices, the effect of interactions was already considered but using weak coupling and mean-field approximations [20], as well as its realization in optical lattices [21, 22] and in LaAlO$_3$/SrTiO$_3$ (111) quantum wells [23]. Bulk oxides with the general chemical formula $A_4B'_2B''_2O_{12}$, such as Ba$_4$CoRe$_2$O$_{12}$ [24], contain trilayers that when seen “from above” also resemble a dice lattice.

In this publication, we study ribbons of the dice lattice. As explained below, we refer to these ribbons as “ladders” borrowing the language of correlated electron systems. We use three primary boundary conditions to achieve our goals: (i) cylindrical geometry, with periodic boundary conditions (PBC) in the short direction and open boundary conditions (OBC) in the long one; (ii) torus geometry, with PBC in both directions; (iii) open geometry, with OBC in both directions. The latter is important to visualize in real space the edge currents and edge charge localization. Because our primary goal is to pave the way towards the future introduction of correlation effects— as discussed below—twisted boundary conditions and associated average over many edge angles were not used, because such procedure would be too demanding in CPU time when including a Hubbard $U$.

Using the three boundary conditions described above, we unveiled a rich eigenvalue spectrum that, surprisingly, continues displaying flat bands even into the smallest ladders we have studied. Moreover, all the geometries studied here display a nonzero Hall conductance in the flat bands region, with the particular value of the 4-leg ladder
system at the Fermi level being very close to \( C = 2 \) as in the planar dice lattice. Moreover, edge currents and edge charge localization appear clearly in all the ladders near zero energy, even in the smallest \( N \times 2 \) cluster, when using both OBC\( \times \)OBC and OBC\( \times \)PBC. Thus, we conclude that even the smallest dice ladders display properties that resemble the two-dimensional topologically nontrivial system [25, 26]. Note that sharp topological numbers, such as integer Chern numbers, cannot be obtained using dice ladders because of the finite number of momenta in the short direction when using cylindrical or fully periodic boundary conditions that prevents a smooth definition of the momentum derivatives involved in the integral that defines \( C \). However, we will show that all properties of the dice lattices are at least qualitatively similar to those of the truly topological two-dimensional systems, as explained above, and in these regards dice lattices are useful “toy models” for dice planes.

The influence of correlation effects is the main current frontier in topological systems [27] and the study of dice ladders paves the way to future investigations where correlation among electrons is incorporated together with flat bands and edge states. How are these flat bands and edge states affected by the introduction of Hubbard \( U \) repulsion? Can new nontrivial phases be generated increasing \( U \)? However, incorporating all these effects in a single many-body study is certainly a challenge [27]. This is particularly important if the technical approach is computationally accurate, a crucial request to obtain unbiased information about the ground state properties of the system. Even for non-topological correlated systems, such as high critical temperature superconductors, achieving accurate predictions for complex models with many competing couplings is difficult. Using mean-field approximations, such as Hartree Fock or other more sophisticated mean-field variations, provides a useful starting point. However, eventually in these complex systems it is important to study special regimes of couplings and lattice geometries where the computational results are nearly exact to compare against results in other more difficult regimes that necessarily must be approximate. A successful strategy followed in cuprates and pnictides/selenides superconductors was to reduce the two dimensionality to the geometry of \( N \)-leg ladders. In this geometry techniques such as the Density Matrix Renormalization Group (DMRG) [28], can achieve considerable accuracy. In particular, recent experimental and theoretical work showed that real two-leg ladder iron-based materials, such as \( \text{BaFe}_2\text{S}_3 \) [29, 30], turn superconducting with high pressure and display nontrivial magnetic properties [31–33]. In Cu-oxide ladders, similar success was theoretically and experimentally achieved [34–36]. As a consequence, exploring the physics of interacting \( N \)-leg dice ladders can be a fertile area of research. But first it is crucial to establish that important properties, such as flat bands and edge currents, survive the transition from planes to ladders. This is the main goal of our publication.

The organization of the manuscript is as follows. In Sec. II, the model and methodology used will be introduced, as well as the main observables calculated. Section III contain the main numerical results with regards to density-of-states and flat bands, starting with the \( N \times N \) cluster, followed by the \( N \times 4 \) ladder, and then the \( N \times 3 \) and \( N \times 2 \) ladders. Section IV addresses the edge currents, edge charge localization, and Hall conductance. Conclusions are provided in Sec. V.

II. MODEL AND METHOD

A. Hamiltonian

In this manuscript, we consider the Hamiltonian studied before in Ref. [10] where those authors used a two-dimensional geometry and worked in momentum space.
This Hamiltonian consists of three components: \( H = H_K + H_{SOC} + H_B \), where \( H_K \) is the tight-binding kinetic energy term, \( H_{SOC} \) is the Rashba spin-orbit coupling, and \( H_B \) the interaction of electrons with an external magnetic field. The kinetic term \( H_K \) is defined as

\[
H_K = -t \sum_{\mathbf{r}, \alpha, \alpha'} \left( c^\dagger_{\mathbf{r}, \alpha, \sigma} c_{\mathbf{r}', \beta, \sigma} + h.c. \right) - \epsilon \sum_{\mathbf{r}} n_{\mathbf{r}, 2},
\]

where \( \mathbf{r}, \mathbf{r}' \) are the unit cell indexes \( [\mathbf{r} = (r_1, r_2)] \) is a vector with components in a coordinate system defined using the unit vectors in Fig. 1, \( \alpha \) and \( \beta \) are the site indexes within the unit cell \( \mathbf{r} \) and \( \mathbf{r}' \), respectively (with \( \alpha, \beta = 1, 2, 3 \)), and \( \sigma = \uparrow, \downarrow \) is the z-axis spin projection of the electron at site \( \alpha \) within the unit cell \( \mathbf{r} \). The on-site energy is \( \epsilon \) and 

\[ n_{\mathbf{r}, \alpha} = \sum_\sigma c^\dagger_{\mathbf{r}, \alpha, \sigma} c_{\mathbf{r}, \alpha, \sigma} \]

is the local density of electrons at site \( \alpha \) in the unit cell \( \mathbf{r} \). The on-site energy affects only the “red” sites of Fig. 1 (those with coordination 6). This kinetic term depicts the inter- or intra-unit cell electronic tunneling between nearest-neighbor sites \( \mathbf{r}, \alpha \) and \( \mathbf{r}', \beta \) with hopping amplitude \( t \). In this article, \( t \) is the energy unit. The electronic density is half-filling i.e. one electron per site.

The Rashba-SOC term in the Hamiltonian is

\[
H_{SOC} = -\lambda \sum_{\mathbf{r}, \alpha, \beta, \sigma, \sigma'} \left( c^\dagger_{\mathbf{r}, \alpha, \sigma} (\hat{D}_{\alpha \beta} \tau)_{\sigma \sigma'} c_{\mathbf{r}', \beta, \sigma'} + h.c. \right),
\]

where \( \lambda \) is the coupling constant \( \lambda \) for all the bonds. The hopping is only between nearest-neighbor sites.

The last term of the Hamiltonian is the interaction of the spin of electrons with a magnetic field

\[
H_B = -B \sum_{\mathbf{r}, \alpha, \sigma, \sigma'} \tau_z^{\sigma \sigma'} c^\dagger_{\mathbf{r}, \alpha, \sigma} c_{\mathbf{r}, \alpha, \sigma'},
\]

where \( B \) is the strength of the magnetic field, acting perpendicular to the plane of the lattice along the \( z \)-direction. This magnetic term breaks the time-reversal symmetry of the Hamiltonian. The Hamiltonian still has translational invariance.

In momentum space, the Hamiltonian becomes

\[
H(k) =
\begin{pmatrix}
-B & 0 & -t \gamma_k^+ & -i \lambda \gamma_k^+ & 0 & 0 \\
0 & B & -i \lambda \gamma_k^- & -t \gamma_k^- & 0 & 0 \\
-t \gamma_k^+ & i \lambda \gamma_k^- & -\epsilon - B & 0 & -t \gamma_k^+ & i \lambda \gamma_k^+ \\
i \lambda \gamma_k^+ & -t \gamma_k^+ & 0 & -\epsilon + B & i \lambda \gamma_k^- & -t \gamma_k^- \\
0 & 0 & -t \gamma_k^- & -i \lambda \gamma_k^- & -B & 0 \\
0 & 0 & -i \lambda \gamma_k^+ & -t \gamma_k^+ & 0 & B \\
\end{pmatrix}
\]

after the Fourier transform \( c^\dagger_{\mathbf{r}, \alpha, \sigma} = \frac{1}{\sqrt{3N}} \sum_k e^{ik \mathbf{r}} e^\dagger_{\mathbf{r}, \alpha, \sigma} \) is used, with \( N (M) \) the number of points in the long (short) direction. We defined \( \gamma_k = 1 + e^{ik \mathbf{r}} + e^{ik' \mathbf{r}} \), and \( \gamma_k^+ = 1 + e^{(k_1 \pm 2\pi/3)} + e^{(k_2 \pm 4\pi/3)} \), where the components are along the axes indicated in Fig. 1 as \( k_i = k_i \hat{e}_i \). The annihilation operator basis is \( (\mathbf{r}, 1), (\mathbf{r}, 2), \mathbf{k}, (\mathbf{r}, 1), (\mathbf{r}, 2), \mathbf{k}, (\mathbf{r}, 1), \mathbf{k}, (\mathbf{r}, 2), \mathbf{k} \) \). This matrix can be diagonalized and the bands are shown in Fig. 2: (a) in the absence of spin-orbit coupling and magnetic field, there are three bands, where one is totally flat and touching another at the \( K \) point, as remarked in [10]; (b) with nonzero \( \lambda \) and \( B \) the original three bands split into six, with the Chern numbers (see definition in Appendix B) as indicated.

![FIG. 2: Energy bands for the \( N \times N \) dice lattice diagonalizing the 6×6 Hamiltonian matrix Eq.(4) in momentum space. (a) are results for \( \lambda = B = 0 \), while (b) are for \( \lambda = 0.3t \) and \( B = 0.2t \). In both cases, \( \epsilon = 0.6t \).](image)

### B. Observables Calculated

#### 1. Currents

The charge current operators can be defined as the sum of two terms, \( J_{ij} \) and \( J_{ij}^{SO} \), known as the spin preserving and spin flipping currents, respectively [37]. The first has a canonical form and arises from the kinetic energy term, while the second originates in the Rashba term and vanishes if \( \lambda = 0 \). We strictly followed the local conservation of charge current to derive the explicit form of these operators. Details of the calculation of these charge current operators are provided in Appendix A.

#### 2. Hall Conductance

From the currents, we computed the transverse Hall conductance (\( \sigma_{xy} \)), described by the Kubo formula as
recently studied in Ref. [38]:

\[ \sigma_{xy} = \frac{2\pi}{N_s} \sum_{\varepsilon_m \neq \varepsilon_n} \frac{f_m - f_n}{\varepsilon_n - \varepsilon_m} \text{Im} (J_{\hat{e}_1 mn} J_{\hat{e}_2 nm}), \quad (5) \]

where \( J_{\hat{e}_1} \) and \( J_{\hat{e}_2} \) are the current operators calculated along the lattice vectors \( \hat{e}_1 \) and \( \hat{e}_2 \), respectively. \( J_{\hat{e}_1 mn} = \langle m | J_{\hat{e}_1} | n \rangle \) is the \( nn' \) matrix element of the current operator \( J_{\hat{e}_1} = J_{\hat{e}_1}^K + J_{\hat{e}_1}^{SO} \). \( N_s = 3MN \) is the total number of sites, \( f_m = (1 + e^{-\beta(\varepsilon_m - \mu)})^{-1} \) is the Fermi function, and \( \zeta \) is the relaxation parameter. \(|n\rangle\) refers to the eigenstates of the full Hamiltonian, which in most of the calculations below will be in a real-space basis.

3. Spectral Function

The definition of one-particle spectral function used in our calculation employs only momenta along the axis 1 that will remain “long” in our ladders, while axis 2 will be short. Specifically, we use the formula

\[ A(k_1, \omega) = \frac{1}{N} \sum_{r_1, r_2, \alpha, \sigma} e^{i k_1 (r_1' - r_1)} \Psi_m^{\dagger}(r_1, r_2, \alpha, \sigma) \Psi_m(r_1', r_2, \alpha, \sigma) \delta(\omega - E_m), \quad (6) \]

where \( r_1 \) (\( r_2 \)), \( r_1' \) are the unit cell indices along the lattice vector \( \hat{e}_1 \) (\( \hat{e}_2 \)). Here, \( k_1 = \frac{2\pi n_1}{N} \) is the momentum along \( \hat{e}_1 \), where \( n_1 = 0, \cdots, N - 1 \), and \( N \) is the number of sites along the long direction of our ladders. \( m \) is the eigenvector index with energy \( E_m \), and we define the amplitude \( \Psi_m(r_1, r_2, \alpha, \sigma) = \langle r_1, r_2, \alpha, \sigma | m \rangle \). We provide width to the delta functions \( \delta(\omega - E_m) \) via a Lorentzian function \( \frac{1}{\pi (\omega - E_m + \eta^2)} \), where \( \eta \) is the broadening of this function.

III. RESULTS

A. \( N \times N \) System

We start with a cluster that resembles the two-dimensional dice system but is finite in both directions. This provides a test that working using a finite lattice can properly reproduce the results already established in Ref. [10] for the bulk dice lattice, as described in the Introduction. We first study the eigenvalues obtained by discretizing momentum space, as it occurs for a finite system, and later we will move into more real-space perspectives and calculations of relevance for this problem, such as edge currents.

\[ \begin{align*}
\text{(a)} & \quad \text{Sketch of a } N \times N \text{ cluster. In this illustration } N = 5 \text{ (focus on the red sites to count unit cells). (b) Bands derived from a } 24 \times 24 \text{ cluster (PBC×PBC) using Eq. (4), at SOC strength } \lambda = 0.3t \text{ and magnetic field } B = 0.2t. \text{ Shown are } 24 \times 6 \text{ bands, with the } 6 \text{ arising from } 3 \text{ sites in the unit cell times a factor } 2 \text{ produced by the magnetic field split. Each band has } 24 \text{ points, joined by interpolating lines. (c) Density-of-states derived from (b) by summing over } k_1. \text{ Note the sharp peaks near zero energy associated with near flat bands in the density-of-states, as it occurs in the bulk system in Fig. 2 (b). The other dispersive bands are associated with the upper and lower bands in Figs. 2 (a,b).}
\end{align*} \]

In Fig. 3 (a), we show a small typical two-dimensional dice cluster. The dangling sites shown have indeed such a character (singular points) when OBC are used, but for PBC in both directions all sites are equivalent i.e. blue and red dots have the same connectivity all over the lattice for PBC×PBC. In panel (b), a \( 24 \times 24 \) cluster is diagonalized. We use the perspective of the direction “1” which will become the “long” (or leg) direction for dice ladders. Thus, in panel (b) \( 24 \times 6 \) bands are shown, as explained in the caption. The density-of-states (DOS) is in panel (c). The results are remarkably close to those implied from Fig. 2 (b), particularly with regards to the crucial two flat bands near zero energy. In the DOS upper and lower dispersing bands, only small spikes in the density-of-states are the remnants of the finite-size cluster used. In summary, a \( 24 \times 24 \) PBC×PBC cluster is sufficient to capture the essence of the dice lattice, as will also be shown below with regards to the edge currents as well.
FIG. 4: (a) Sketch of a $N \times 4$ ladder. In the example shown $N$ is 8 (focus on the red sites to count unit cells). (b) Bands are derived from a $150 \times 4$ cluster (PBC×PBC) diagonalizing Eq.(4) at SOC strength $\lambda = 0.3t$ and magnetic field $B = 0.2t$. Shown are $4 \times 6 = 24$ bands, with the factor 6 explained in the caption of Fig. 3. (c) Density-of-states derived from (b) by summing over $k_1$. Note the 6 sharp peaks associated with near flat bands, 2 of which are isolated near zero energy (the important ones), while 4 are mixed with other non-flat bands.

B. $N \times 4$ Ladder

Now we turn to a dice ladder with 4 unit-cells along the short direction. A sketch is shown in Fig. 4 (a). Note that because we have a unit cell with three sites, effectively there are 12 lines of sites, with a vertical periodicity blue-blue-red. This shows that numerically the effort to study these ladders after adding electronic interactions would be harder than the nominal size suggests. Specifically, a $N \times 4$ dice ladder costs in practice a similar effort as a $N \times 12$ one-orbital Hubbard model ladder from, e.g., the DMRG perspective.

With regards to the relevance of dice ladders to mimic planes, what is remarkable are the results in Figs. 4 (b,c). In spite of the very different lengths in both directions, panels (b,c) have clear similarities with Figs. 3 (b,c). In particular, both display the flat bands near zero energy, almost identical in both cases. To the extent that one of the primary non-trivial aspect of dice lattices are the flat bands, then the $N \times 4$ ladder keeps that aspect intact. In addition, surprisingly, there are other flat bands in this 4-leg ladder, 2 in the original upper-energy dispersing region and 2 in the lower-energy region. However, these bands are not isolated from the rest, even with a nonzero spin-orbit coupling and magnetic field. Thus, their value in inducing non-trivial properties of the system are questionable. For this reason, we will not focus on those extra flat bands. However, we remark again that we found flat bands near zero energy, successfully confirming that a 4-leg dice ladder resembles the two-dimensional system.

Moreover, following the procedure outlined in the Appendix based on Ref. [39] we have calculated the Chern number of the near-zero energy flat bands of the 4-leg dice ladder. As explained in the introduction, ladders are not expected to have sharp topological properties because of their discrete nature in one direction. However, remarkably, we found $C \sim 2$ and $C \sim -2$ for the two flat bands as in Fig. 2 (b). For details, see below and Appendix B. In essence, the $N \times 4$ ladder has basically the same properties as the two-dimensional dice lattice.

C. $N \times 3$ System

Consider now 3-leg dice ladders of size $N \times 3$, such as illustrated in Fig. 5 (a). As explained before, the effective number of “legs” of the 3-leg dice ladder, of relevance for future computational work in real-space when adding interactions, is 9 because each unit cell has 3 sites. As in the previous case of a 4-leg ladder, in panel (b) we present momentum-space results using $k_1$ in the horizontal axis (long direction). This provides a discrete set of bands
because of the finite number of unit cells along the short direction (see detail in caption). But once again, the flat bands near \( E = 0 \) remain solidly in place. Actually the density-of-states is still qualitatively similar to the two-dimensional dice lattice cluster Fig. 3 (c). In this case, there are no extra flat bands away from the vicinity of Fermi energy zero, as found with 4-legs, suggesting that the existence of these extra features may depend on whether we have an even or odd number of unit cells along the short direction.

![Image of a ladder](image)

**FIG. 6:** (a) Sketch of a \( N \times 2 \) ladder. In the example shown \( N \) is 8 (focus on the red sites to count unit cells). (b) Bands derived from a 150×2 cluster (PBC×PBC) diagonalizing Eq.(4) at SOC strength \( \lambda = 0.3t \) and magnetic field \( B = 0.2t \). Shown are 12 bands i.e. 2×6, as explained in the caption of Fig. 3. (c) Density-of-states derived from (b) by summing over \( k_1 \). Note the 6 sharp peaks in the density-of-states associated with near flat bands, 2 of which are isolated near zero energy, while 4 are mixed with other non-flat bands.

**D. \( N \times 2 \) System**

Finally, we arrived to the “shortest” ladder studied here: the 2-legs dice ladder. This ladder, when considered in terms of the number of legs along the short direction, has 6 legs in the one-orbital Hubbard analog, as illustrated in Fig. 6 (a). Thus, this system is accessible to present computational efforts using DMRG. For this reason, the 2-leg ladder is particularly important.

In Fig. 6 (b) the bands plotted vs \( k_1 \) are shown, as before for 3- and 4-leg ladders. Once again, remarkably, the flat bands near energy zero are clearly present, even in this “shortest” system studied here. Similarly as in the case of 4 legs, extra flat bands were identified immersed in the upper- and lower-energy regions, but they are not of our interest. The density-of-states in Fig. 6 (c) now are different from the two-dimensional cluster Fig. 3 (c) with regards to the upper and lower energy regions, due to the extra flat bands. But with regards to the region near zero energy, all systems \( N \times N, N \times 4, N \times 3, \) and \( N \times 2 \), behave similarly: they all have similar flat bands in this energy region.

![Image of charge current](image)

**FIG. 7:** Charge current \( \langle J_{\hat{e}_1} \rangle \) (red dots, left axes) in an OBC×PBC system shown vs the unit cell index \( r_1 \) along the long axis \( \hat{e}_1 \) for different dice ladders. Electronic density (blue dots, right axes) corresponding to the in-gap states i.e. states between the two flat bands near zero, with the gap among them generated by the magnetic field. These in-gap states are induced by using cylindrical boundary conditions. The density result is an average over the four in-gap states closest to zero energy. The location of both current and charge suggests these in-gap states are edge states. Shown are averages over the short direction \( r_2 \) (of course in cylindrical geometries the results are translationally invariant along this PBC direction). Panels (a), (b), (c), and (d) are for ladder sizes \( 30 \times 30, 60 \times 4, 60 \times 3, \) and \( 60 \times 2 \), respectively. The parameters used in all panels are: \( \lambda = 0.3t, B = 0.2t, \epsilon = 0.6t \). Note that for the smaller ladders with 3 and 2 legs, the edge state penetrates one unit cell deeper into the cylinder than the rest, which is just a small effect.

**IV. EDGE CURRENTS AND EDGE STATES**

**A. Cylindrical Boundary Conditions**

To study the properties of the dice ladders we have carried out several other calculations in addition to the DOS and their flat bands. For example, using cylindrical boundary conditions, with PBC along the short direction and OBC along the long direction, we searched for edge
currents at the edges of this geometry. Results are shown in Fig. 7. At the center of the cylinders – away from the edges – there are no currents, but at the edges currents develop with opposite senses of circulation. What is remarkable is the obvious similarity, both qualitatively and quantitatively, between the $N \times N$ cluster that mimics well the two-dimensional plane, panel (a), and the dice ladders in panels (b,c,d): they all behave almost identically, with edge currents circulating in the same direction and of the same magnitude. This confirms that the interesting edge currents of two dimensional dice lattices in cylinders also appear in the dice ladders.

The use of cylindrical boundary conditions creates in-gap states in between the flat bands, whose gap was opened by the magnetic field. Studying the wave function of those in-gap states, we calculated the electronic density. The results are also shown in Fig. 7, with details in the caption. As intuitively expected, these in-gap states are indeed edge states, associated with the edge currents.

**B. Open Boundary Conditions in Both Directions**

1. **Edge Currents in $N \times N$ System**

As further test of the reliability of using finite systems to address the topology of dice lattices, in Fig. 8 we have calculated the charge current for the case of OBC along both directions, in the presence of both spin-orbit coupling and an external magnetic field. We use a cluster that mimics the two-dimensional systems, namely with the same number of unit cells along both directions. In Fig. 8 it is obvious to the eye that edge currents develop for a 12×12 cluster, as expected. We have confirmed the same for up to 30×30 clusters, but displaying the smaller system 12×12 as illustration provides better clarity to the readers. The dangling sites, unavoidable in OBC×OBC geometries, have zero current, obvious due to current conservation. In fact, we confirmed explicitly charge conservation at every site of the lattice as a test of our codes. In the two vertices without dangling sites, the current is more extended into the bulk than at the straight line edges where the currents are very confined to the frontier. Intuitively, this makes sense due to the sudden direction change of the current.

2. **Edge Currents in $N \times 4$, $N \times 3$, $N \times 2$ dice ladders**

For the 4-, 3-, and 2-leg dice ladders, the situation is similar as in the symmetric $N \times N$ cluster: in all cases there are sharply-defined edge currents, as shown in Fig. 9. A technical detail is worth remarking: as we reduce the number of legs we have to adjust the $\lambda$ and $B$ parameters to better achieve the confinement of current to the edges. Without this minor parameter adjustment, the edge currents moving left and right, along the two
horizontal edges, may develop a non-negligible overlap because they have a finite size near the edge, and then current distortions occur. However, even though in some regions of parameter space the edge currents are not as crisp as in Fig. 9 due to overlaps, in all cases investigated the sense of rotation of the currents is always the same and their existence is not in doubt. In summary, all ladders behave very similarly to planes when OBC conditions are used along both directions: in all cases clear edge currents develop.

**FIG. 9**: Charge current calculated at each lattice bond for different ladder sizes. In (a) the system size is 30×4 while the parameters chosen are $\lambda = 0.3t$, $B = 0.2t$, and $\epsilon = 0.6t$. In (b) the system size is 30×3, with parameters $\lambda = 0.3t$, $B = 0.25t$, and $\epsilon = 0.6t$. In (c) the system size is 30×2 with parameters $\lambda = 0.1t$, $B = 0.4t$, and $\epsilon = 0.6t$. All plots are using boundary conditions OBC×OBC. The presence of well-defined edge currents is clear in the three ladders.

3. **In-gap edge states with OBC×OBC**

There are two other important aspects to test next. In topological systems, using open boundary conditions in both directions leads to the previously described edge currents in real space, but also to related crossings of bands in momentum space. Moreover, the Chern number is associated with the number of those crosses in planar systems where the Chern number is well defined. It is interesting to study what occurs now in dice ladders.

In Fig. 10 we show the bands obtained from the one-particle spectral function $A(k_1, \omega)$ for the case of OBC×OBC (technical aspects were already explained in observables Sec. II.B). We will focus on the energy domain where the flat bands develop near zero energy. For PBC×PBC, these figures simply display two nearly flat bands with no extra features due to the absence of edges. But with OBC×OBC in our finite but large clusters we clearly observe the development of edge states that manifest as crossing points. The similarity between the $N \times N$ cluster [panel (a)] and all the rest of the ladders [panels (b,c,d)] is remarkable. In all cases, the presence of two crossing points in principle indicates Chern number $C = 2$, in agreement with the conclusions of previous sections. As explained before, for the dice ladders we do not expect a perfect quantization to an integer of the Chern number calculation due to the few momentum-space points available along the short direction. However, the conclusion that all cases panels (a,b,c,d) share similar features is unavoidable simply inspecting by eye. All these results suggest that two chiral edge states exist both in the dice plane and ladders, even though the Chern number is not well defined for ladders.

For completeness, and as with the edge states for cylinders, we warn the reader that for the 3- and 2-legs dice ladders we observed that for other sets of $\lambda$ and $B$ parameters, a small gap opens at zero energy where the crossings appear in Figs. 10 (c,d) (for 4-legs the gaps are so small that are not visible in the scale of the figure). In the presence of those gaps, edge states were nevertheless observed for 3- and 2-legs suggesting that there is an effective mass in the associated chiral modes. This subtle matter will be investigated in future work.

Figure 11 shows the electronic density corresponding to the range of energies where the levels cross in Fig. 10 (i.e. the in-gap states). In agreement with expectations for the two-dimensional lattice, panel (a), for the dice ladders the various panels (b-d) also show that in the range of energy near the middle of the gap between flat bands, the states generated by using OBC×OBC are indeed confirmed to be “edge states” as manifested by the localization of charge at the edges.
number for the flat bands near zero energy in two dimensions. For the case of PBC×PBC, not shown, after entirely crossing the first lower flat band, $\sigma_{xy}$ remains constant, and then it decreases when reaching the second band that has the same Chern number but of opposite sign. For OBC×OBC, the existence of the edge states levels in between the flat bands makes $\sigma_{xy}$ to evolve smoothly in value in between the flat bands, as opposed to having a plateaux. Overall, all the clusters studied, both the symmetric $N \times N$ and the dice ladders, share a qualitative similar behavior in the Hall conductance.

**FIG. 10:** Left panels (a), (b), (c) and (d): the one-particle spectral function $A(k_1, \omega)$ vs $k_1$ for various clusters, using OBC×OBC. For all these $A(k_1, \omega)$ plots we used broadening $\eta = 0.004t$ and energy resolution $d\omega = 0.02t$ in the vertical axis. Right panels (e), (f), (g) and (h): the corresponding Hall conductance $\sigma_{xy}$, again for OBC×OBC and the same set of parameters as on the left. For all the $\sigma_{xy}$ plots we used broadening $\zeta = 0.05t$. Parameters chosen for (a) and (e) are $\lambda = 0.3t$, $B = 0.2t$, and $\epsilon = 0.6t$, and cluster size $30 \times 30$. In (b) and (f) the parameters are $\lambda = 0.3t$, $B = 0.2t$, and $\epsilon = 0.6t$, with the cluster size used for $A(k_1, \omega)$ being $60 \times 4$ and for $\sigma_{xy}$ we chose $300 \times 4$ to smooth out size effects. In (c) and (g), parameters are $\lambda = 0.7t$, $B = 0.2t$, and $\epsilon = 0.6t$, with cluster size for $A(k_1, \omega)$ $60 \times 3$ and for $\sigma_{xy}$ $300 \times 3$. In (d) and (h), parameters are $\lambda = 0.5t$, $B = 0.2t$, and $\epsilon = 0.6t$, with cluster size for $A(k_1, \omega)$ $60 \times 2$ and for $\sigma_{xy}$ $300 \times 2$.

**FIG. 11:** Electronic density adding the contributions from all the “edge states” generated by using OBC×OBC—in between the two flat bands near zero energy—more specifically within the range of energy $\Delta\omega = 0.2t$ from $\omega = -0.1t$ to $0.1t$. The radius of each circle is proportional to the value of the density. These states, that also generate the edge currents shown in previous figures, are clearly localized at the edge, as expected. Parameters are the following: (a) $12 \times 12$ cluster, $\lambda = 0.3t$, $B = 0.2t$, and $\epsilon = 0.6t$; (b) $30 \times 4$, $\lambda = 0.3t$, $B = 0.2t$, and $\epsilon = 0.6t$; (c) $30 \times 3$, $\lambda = 0.7t$, $B = 0.2t$, and $\epsilon = 0.6t$; (d) $30 \times 2$, $\lambda = 0.5t$, $B = 0.2t$, and $\epsilon = 0.6t$.

4. **Hall conductance**

On the right panels of Fig. 10, the Hall conductance is shown in the same range of energy as on the corresponding left panels. In Fig. 10 (e), clearly we observe the growth of $\sigma_{xy}$ with increasing energy, starting from negative energy, when the first flat band is reached. This is to be expected because of the nonzero value of the Chern

With respect to the specific value they reach at the central energy $\epsilon_F = 0$, for the $N \times N$ cluster the value $\sim 1.75$ is close to the expected 2. In fact for PBC×PBC it is even closer, being approximately 1.9. Size effects are to be expected and by extrapolation to large $N$, we conclude that the Chern number for the $N \times N$ cluster is indeed very close to 2 within our accuracy. For the dice
ladders, systematically the zero energy Hall conductance is smaller, although they are all qualitatively similar. In all cases, the $\epsilon_F = 0$ value is larger than 1.

Extrapolating to large $N$ the results for the $N \times 4$ ladder gives a number also close to 2, as in the planar cluster, confirming once again that 4-leg ladders are virtually identical to planes. But for the $N \times 3$ and $N \times 2$ dice ladders the extrapolation is smaller than 2. This is not surprising since, as explained before, the dice ladders are not expected to display an integer as Chern number in their bands due to the discrete momentum in the short direction. However, once again, qualitatively even the shortest ladders do resemble the planar clusters in all respects we have studied.

In Fig. 12 the Hall conductance at the Fermi energy is shown vs broadening for the case of PBC×PBC where size effects are less severe. The extrapolations to zero broadening discussed in the caption provide two alternative paths to such extrapolation. For the 24×24, it appears that $C = 2$ is a solid conclusion, in excellent agreement with expectations. For the case of the 4-leg ladder, the results also suggest $C \sim 2$ although certainly a more careful procedure should be followed if a precise number is desired. As explained several times, we do not expect the Chern number to behave exactly similarly in dice ladders as in dice planes, but the results shown are sufficient to illustrate that the 4-leg ladder is virtually identical to the two-dimensional system in every respect. However, for the case of 3-leg dice ladders, the deviations are pronounced and it seems unlikely $C$ will extrapolate to 2. Similarly, the case of the 2-leg ladder is even more pronounced, with a $C$ close to 1. For 3- and 2-leg ladders, the edge currents moving in opposite directions may start overlapping, distorting the effects found in planes. Yet, all of the dice lattices we studied have systematic behavior similar to one another.

![Graph](image)

FIG. 12: Hall conductance ($\sigma_{xy}$) at the Fermi level ($\epsilon_F = 0$) vs the relaxation parameter $\zeta$ for PBC×PBC clusters of sizes (a) 24×24, (b) 100×4, (c) 200×3, and (d) 300×2, all for the same parameters $\lambda = 0.3t$, $B = 0.2t$, and $\epsilon = 0.6t$. (a,b,c) share the vertical axis on the left, while (d) has its own vertical axis on the right. The extrapolation to zero broadening can be performed using all the red dots data or instead the dashed line shown employing only broadenings above 0.1t. The reason is that the systematic development of a negative curvature in the data, deviating from a straight line, could be a size or broadening effect. In panel (a) clearly both extrapolating via all the red dots or only using those leading to the dashed line suggest a convergence very close to the expected $C = 2$.

V. CONCLUSIONS

In this publication we have studied the dice lattice when geometrically reduced from the standard planar geometry to ladders. These ribbons are here called “ladders” by analogy to the physical systems widely studied in other contexts, such as high critical temperature superconductors. The Hamiltonian used is the same as employed before in Ref. [10], namely with a tight-binding term, Rashba spin-orbit coupling, on-site energies, and an external magnetic field. We have focused on several non-trivial quantities of relevance in two dimensions, such as the existence of flat bands near the Fermi level, the presence of edge currents when using OBC, the observation of localized charge at the edges near zero energy in the one-particle spectral function also when using OBC, and a nonzero Hall conductance. The remarkable conclusion of our effort is that all systems studied, even the smallest 2-leg ladder, display common properties suggesting that their qualitative behavior is similar even with the reduction of the size in one direction.

Our effort paves the way towards the introduction of correlation effects, such as the Hubbard repulsion $U$, via accurate computational many-body techniques for one dimension, such as DMRG. For example, even for the smallest 2-leg ladder, the evolution of the prominent edge currents and flat bands with increasing Hubbard $U$ strength is interesting and can be studied, both for OBC×OBC and OBC×PBC, the latter with PBC along the short direction. In the near future, calculations involving both topological-like aspects and correlation effects will be presented using dice ladders.
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APPENDIX

A. Charge Current Operators

From the kinetic term of the Hamiltonian and using the continuity equation for the charge, the following current operators were derived:

$$ J_{j 	o i_p}^K = J_{j 	o i_p, \uparrow \downarrow}^+ + J_{j 	o i_p, \downarrow \uparrow}^- $$  \hspace{1cm} (7)

where \(i_p\)'s are the six neighboring sites of site \(j\) as shown in Fig. 13 with \(p = 1, \ldots, 6\). The current operator used above is defined as

$$ J_{j 	o i_p, \sigma 	o \sigma'} = -i \left( c_{i_p, \sigma}^\dagger \sigma_j,\sigma - \text{h.c.} \right) $$

FIG. 13: Rashba-SOC lattice connections from the six-coordination site \(j = (r,2)\), as example. The green arrows depict the SOC vectors \(\hat{D}_{ij}\) for the bonds connected to \(j\). \(\hat{e}_1\) and \(\hat{e}_2\) are the lattice unit vectors. 1, 2 and 3 are the site labels within a unit cell \(r\). Following [10], X, Y and Z are the axes of the spin space used for the Rashba connections: the Y direction is parallel to the line from (r,2) to (r,3), and the X direction is perpendicular.

Similarly, from the SOC term of the Hamiltonian, the following charge current operators were derived:

$$ J_{j 	o i_p}^{SO} = J_{j 	o i_p, \uparrow \downarrow}^+ + J_{j 	o i_p, \downarrow \uparrow}^- $$  \hspace{1cm} (8)

where

$$ J_{j 	o i_p, \sigma 	o \sigma'} = \lambda \left( c_{i_p, \sigma}^\dagger \sigma_j,\sigma \sigma_j,\sigma + \text{h.c.} \right), $$

and here \(\sigma \neq \sigma'\).

The total charge current from site \(j\) to one of the neighboring sites \(i_p\) is:

$$ J_{j 	o i_p} = J_{j 	o i_p}^K + J_{j 	o i_p}^{SO}. $$  \hspace{1cm} (9)

These definitions of charge currents satisfy the conservation property (both locally and globally).

B. Chern Number

The Chern number for the \(n^{th}\) band is defined in the continuum as:

$$ C_n = \frac{1}{2\pi} \int_{T^2} F_{12}(k) dk, $$  \hspace{1cm} (10)

where \(F_{12}(k) = \partial_1 A_2(k) - \partial_2 A_1(k)\) is the Berry curvature, and \(A_{\mu}(k) = \langle u_{n,k} | \partial_{\mu} | u_{n,k} \rangle\) is the Berry connection. \(T^2\) is the surface of a Torus formed by considering periodic boundary condition (PBC) in both the \(\hat{e}_1\) and \(\hat{e}_2\) directions. \(\partial_{\mu} = \partial / \partial k_{\mu}\) is the partial derivative with respect to momentum \(k_1\) and \(k_2\) along the \(\hat{e}_1\) and \(\hat{e}_2\) direction, respectively.

For lattice calculations, the above equations cannot be used unless we find Bloch functions “\((r, \alpha, \sigma | u_{n,k})\)” in a real-space basis. Since our Hamiltonian is translationally invariant, the set of Bloch states \(\{ |r, \alpha, \sigma | \Psi_{n,k}\}\}\) are eigenstates of the Hamiltonian, where \(\Psi_{n,k}(r, \alpha, \sigma) = \langle r, \alpha, \sigma | \Psi_{n,k}\rangle = e^{ik_1 r} u_{n,k} (r, \alpha, \sigma)\), and in second quantization \(\{ |r, \alpha, \sigma\rangle \} = c_{r,\alpha,\sigma}^\dagger \). Note that the set \(\{ |r, \alpha, \sigma | \Psi_{n,k}\}\}\) are orthogonal to each other but not necessarily the set \(\{ \langle r, \alpha, \sigma | u_{n,k}\}\}\) which explains why the Berry connections are (always) non-zero.

Because our computational calculation has been performed primarily in a real-space basis, the eigenstates we obtain are, in general, a superposition of all the Bloch states with the same energy, see Fig. 14. For this reason, we cannot directly use the eigenstates calculated from the diagonalization computer code to find the Chern number.

To solve this issue, consider a computer generated real-space eigenstate \(|m\rangle\) with energy \(E_m\). This state is a linear combination of the real-space site basis, i.e., \(|m\rangle = \sum_{r,\alpha,\sigma} C_{r,\alpha,\sigma}(m) |r, \alpha, \sigma\rangle\), where \(C_{r,\alpha,\sigma}(m) = \langle r, \alpha, \sigma | m\rangle\) are the coefficients of the transformation matrix from site basis to the real-space eigenstate of the Hamiltonian.

FIG. 14: \(E_m\) vs \(k_1\) sketch illustrating how we computed \(\langle r, \alpha, \sigma | \Psi_{n,k}\rangle\) between two non-degenerate non-touching bands (points in blue are explained in the text).
As expressed above, \(|m\rangle\) can also be written as a superposition of all the Bloch states \(|\Psi_{n,k}\rangle\) with the same energy (see Fig. 14) as \(|m\rangle = \sum_{n,k} \Gamma^m_k |\Psi_{n,k}\rangle\), where \(\Gamma^m_k = \langle \Psi_{n,k} | m \rangle\) are the transformation coefficients from Bloch states to real-space eigenstates. From the above equations and considering that \(u_{n,k}(r,\alpha,\sigma) = (r,\alpha,\sigma|u_{n,k}\rangle\) are repeated between unit cells i.e. \(u_{n,k}(r,\alpha,\sigma) = u_{n,k}(r + \mathbf{r}',\alpha,\sigma)\), we calculate: \[
\sum_{r'} (r + \mathbf{r}',\alpha,\sigma|m\rangle e^{-i\mathbf{k}\cdot r'} = \\
= \sum_{n,k',r'} \Gamma^m_k(m)e^{i\mathbf{k}\cdot(r+r')/(r',\alpha,\sigma|u_{n,k}\rangle e^{-i\mathbf{k}\cdot r'}
= \sum_{n,k',r'} \Gamma^m_k(m)e^{i\mathbf{k}\cdot(r+r')e^{-i\mathbf{k}\cdot r'}(r',\alpha,\sigma|u_{n,k}\rangle
= V \sum_n \Gamma^m_k(m)e^{i\mathbf{k}\cdot r}\langle r,\alpha,\sigma|u_{n,k}\rangle
= V \sum_n \Gamma^m_k(m)\langle r,\alpha,\sigma|\Psi_{n,k}\rangle,
\]
where it must be understood that \(|r + \mathbf{r}',\alpha,\sigma) = e^{i\frac{\pi}{2}\mathbf{r}'\cdot\mathbf{a}_2}|0\rangle\), and \(V\) is the volume of the system. We know that Chern numbers are well defined only for non-intersecting energy bands. In our case, with the addition of the Rashba-SOC and the Zeeman field \(\mathbf{B}\) we fulfill this condition. From this physical argument, illustrated in Fig. 14, we know that for fixed momentum \(\mathbf{k}\) and energy \(E_m\), only one value of \(\Gamma^m_k(m)\) is non-zero for a specific band \(n\). Thus, we can write Eq.(11) as:
\[
\sum_{r'} \langle r + \mathbf{r}',\alpha,\sigma|m\rangle e^{-i\mathbf{k}\cdot r'} = V \Gamma^m_k(m) \langle r,\alpha,\sigma|\Psi_{n,k}\rangle
\]
Of course we do not know the specific value of \(\Gamma^m_k(m)\), but Eq.(12) implies that for each individual band \(n\), \(\langle r,\alpha,\sigma|\Psi_{n,k}\rangle \propto \sum_{n,k'} \langle r + \mathbf{r}',\alpha,\sigma|m\rangle e^{-i\mathbf{k}\cdot r'}\), so by calculating \(\sum_{r'} \langle r + \mathbf{r}',\alpha,\sigma|m\rangle e^{-i\mathbf{k}\cdot r'}\) and normalizing it, the Bloch states \(|\Psi_{n,k}(r,\alpha,\sigma) = (r,\alpha,\sigma|\Psi_{n,k}\rangle\) can be obtained in real space for band \(n\). After calculating this Bloch states, now \(u_{n,k}(r,\alpha,\sigma)\) can be obtained using \(\langle r,\alpha,\sigma|u_{n,k}\rangle = e^{-i\mathbf{k}\cdot r}\langle r,\alpha,\sigma|\Psi_{n,k}\rangle\), which can directly be used for the calculation of the Chern number.

Once the Bloch functions are found, we follow the method of Fukui et al. [39], to calculate the Chern number for a discrete lattice. We first compute the U(1) link variables \(U_\mu(k) = \langle u_{n,k}(r,\alpha,\sigma)|u_{n,k+\hat{\mu}}(r,\alpha,\sigma)\rangle / \langle u_{n,k}(r,\alpha,\sigma)|u_{n,k+\hat{\mu}}(r,\alpha,\sigma)\rangle\) as defined in their paper (\(\hat{\mu}\) is a vector along the directions of the lattice vectors \(\hat{e}_1\) and \(\hat{e}_2\) with magnitude \(2\pi/N_\mu\)), from the Bloch functions evaluated above. Then, we calculate the discretized lattice field strength \(F_{12}(k)\) as:
\[
F_{12}(k) = \partial_1 A_2(k) - \partial_2 A_1(k)
= A_2(k + \hat{\mu}_1) - A_2(k) - A_1(k + \hat{\mu}_2) + A_1(k)
\]
where forward discretization of \(\partial_\mu\) was used. Under this approximation, for example,
\[
A_1(k) \approx \langle u_{n,k} u_{n,k+\hat{\mu}_1}\rangle - \langle u_{n,k} u_{n,k}\rangle.
\]
Assuming that all \(\{|u_{n,k}\}\) are normalized to 1, it can be shown that
\[
F_{12}(k) \approx \langle u_{n,k+\hat{\mu}_1} u_{n,k+\hat{\mu}_1+\hat{\mu}_2}\rangle - \langle u_{n,k} u_{n,k+\hat{\mu}_2}\rangle - \langle u_{n,k+\hat{\mu}_2} u_{n,k+\hat{\mu}_1+\hat{\mu}_2}\rangle + \langle u_{n,k} u_{n,k+\hat{\mu}_1}\rangle.
\]

Pictorially, each of these individual terms can be imagined by placing them at the links of a discretized Brillouin zone, as shown in Fig. 15. Moreover, the sign gives a sense of circulation. \(F_{12}(k)\) then becomes a flux variable around an elementary plaquette of the \(k\)-space lattice Then, following the directions [39] to calculate the lattice field strength \(\tilde{F}_{12}(k) = \ln (U_{12}(k)) = \frac{1}{2\pi i} \sum_k \tilde{F}_{12}(k)\) can be computed. The Chern number associated with the \(n\)th band as:
\[
C_n = \frac{1}{2\pi i} \sum_k \tilde{F}_{12}(k).
\]

Note that the magnitude of the quantities inside the lattice field strength \(\tilde{F}_{12}(k)\) is always 1 and thus \(-i\pi < \tilde{F}_{12}(k) < i\pi\).

Following this momentum-space procedure, we calculated the Chern number for the \(N \times N\) clusters, with focus on the flat band below the Fermi level. The results were clearly equal to 2 (not shown). A result \(C \approx 2\) was obtained for the \(N \times 4\) ladder, confirming that these two systems are in practice virtually identical. For the case of 3-leg ladders, however, our results seem to converge to a smaller \(C\), in agreement with the deviations from 2 observed in Fig. 12 (c). For 2-leg ladders, the calculation is not possible due to trivial cancellations arising from the availability of only two momenta along the short direction. Nevertheless, although using \(\sigma_{xy}\) and

FIG. 15: Pictorial representation of the flux variable \(F_{12}(k)\) in a \(k\)-space plaquette.
real-space edge currents is more reliable, the momentum-

space method outlined in this Appendix provides results compatible with those in real space.

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