Shaking driven non-trivial topology in a Floquet-engineered dice lattice

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Starting from a gapless two-dimensional dice system, we aim to design a periodic driving scheme to induce a topologically nontrivial and gapped phase by only tuning the driving strength. The effective Hamiltonian is derived both in real-space and quasi-momentum space. By analyzing the dispersions, we find that there are three separated quasi-energy bands once the driving is applied. The topological phase diagram containing Chern number of the lowest quasi-energy band shows that when the hopping strengths of nearest-neighboring hoppings are balanced, the system persists in the topological non-trivial phases with Chern number $C_1 = 2$ within a wide range of driving strength. Accompanied by the imbalanced nearest-neighboring hopping strengths, there appears a topological phase transition, making Chern number change from $C_1 = 2$ to $C_1 = 1$. This transition is further verified by our analytical method. The non-zero Chern number signals the existence of the edge modes which are intuitively seen in the edge-state spectra. The connection between the Chern number and the edge modes is well interpreted by the principle of the bulk-edge correspondence.

I. INTRODUCTION

The emergence of the non-trivial topology in the band insulators is in relevance with the properties of their band structure. The resulting topological band insulators [1, 2] are not only classified by the symmetries but also are found to be immune to the inhomogeneous perturbations because of their preserved symmetries [3–5]. TKNN theory [6] tells that if a band insulator is capable of changing between the topological trivial and non-trivial phase, there shall exist tunable band inversion points (or say Dirac points), at which bands either are non-degenerate or degenerate. Accordingly, the crucial factor to engineer topological band structures is controlling the degeneracies of the bands at these inversion points [7], which is also a crucial factor to prepare a band insulator with quantum anomalous Hall effect [8, 9]. Nevertheless, in practice, it remains a challenge to realize the flexible control on the band inversion points in experiments [10, 11].

Alternatively, the control of band characteristic can be realized by the Floquet engineering which offer a new way to study the dynamical properties of topological matters [7, 12]. Due to the periodic driving, the intrinsic trivial characteristic of the band structures of the static system changes, forming non-trivial Floquet quasi-energy bands. For decade, the scheme of Floquet band engineering has been employed in solid-state materials [13–18], photonic systems [19, 20], and the ultracold atoms [7, 12, 21–28]. Moreover, this method offers a possibility to induce tunable interactions [29]. Recently, an experimentally and theoretically investigation [30] on the feasibility to individually control the quasi-energy bands coupling and decoupling at band inversion points is carried out in a one-dimensional lattice by tuning the driving strength. Motivated by this Floquet engineering, we want to study whether it is possible to decouple the intrinsic gapless bands and form gaped quasi-energy band structures with non-trivial topology in a driven two-dimensional optical lattice by only tuning the driving strength.

Our driving scheme is performed in a two-dimensional dice lattice [31–33], where there are three types of sublattice sites. The position of the potential is periodically driven in time. We derive the effective model in real space by means of the Floquet analysis [12, 34, 35]. Without driving, particles only hop between nearest-neighbor sites. From the band structure, one can see that bands are gapless at a Dirac points. When periodic driving is introduced, we uncover that the next-nearest-neighbor hoppings between all the same sublattice types are induced, inducing a non-trivial band structure, and forming three separated quasi-energy bands. After numerically and analytically calculating the topological invariant of the lowest quasi-energy band, we find that the system persists in the topological phase with Chern number being $C_1 = 2$ when the applied driving force is within a wide range of parameter space. The large topological invariant indicates the existence of multiple edge states, readily seen in the edge-state quasi-energy spectrum. Furthermore, we find that if the nearest-neighbor hopping strengths are imbalanced, the number of edge modes will decrease, and the resulting Chern number becomes $C_1 = 1$. The correspondence between the Chern number and the edge modes is well interpreted by the principle of the bulk-edge correspondence [36].

II. DICE LATTICE AND THE FLOQUET ENGINEERING

The two-dimensional dice optical lattice formed by the lasers [33] is illustrated in the schematic Fig. 1(a). In each unit cell braided by two primitive lattice vectors, there are three types of sublattice shown by $R$, $B$, and $G$. By considering spinless and non-interacting ultracold fermionic atoms trapped in this lattice, a generalized
The attitude of our Floquet band engineering is to theoretically investigate the feasibility that inducing gapped band structures and preparing non-trivial topological phases can be realized by only tuning the driving strength. Therefore, the driving strength $F$ can ranges from zero to a finite value. We derive the effective Hamiltonian by the Floquet analysis \cite{12, 34, 35}. Transforming the total Hamiltonian to the rotating frame, we have the gauge-transformed Hamiltonian $H_{\text{rot}}$ as (see details in the Appendix A)

$$H_{\text{rot}} = \hat{U}^{-1}(t) \left[ H_{\text{ini}} + \hat{H}_{\text{dri}} \right] \hat{U}(t) - i\hbar \frac{d\hat{U}(t)}{dt} \tag{3}$$

where $\hat{U}(t)$ is the time-dependent gauge transformation operator and $\hat{U}(t) = \exp \left( -\frac{i}{\hbar} \sum_{\alpha_j} \int_0^t V(\mathbf{r}_{\alpha_j}, t') dt' \cdot \hat{n}_{\alpha_j} \right)$.

Our Floquet band engineering is to apply an anisotropic time-dependent shaking force $\mathbf{F}(t)$ on the initial lattice platform with $F \cos(\omega t)$ in the $e_x$ direction and $-F \sin(\omega t)$ in the $e_y$ direction, like the shaking of the Haldane lattice \cite{24}, where $F$ and $\omega$ indicate the strength and the frequency of the shaking force, respectively. The driving force is described by the time-dependent on-site potential $H_{\text{dri}}$

$$H_{\text{dri}} = \sum_{\langle \mathbf{r}_i, \mathbf{r}_j \rangle} t \left( \hat{c}_{\mathbf{r}_j}^{\dagger} \hat{c}_{\mathbf{r}_j} + H.c. \right) + \sum_{\langle \mathbf{g}_i, \mathbf{r}_j \rangle} t_1 \left( \hat{c}_{\mathbf{g}_j}^{\dagger} \hat{c}_{\mathbf{r}_j} + H.c. \right). \tag{1}$$

$H_{\text{ini}}$ describes the hoppings between the nearest-neighbor sites with $\alpha_j \in \{R, G, B\}$ being the coordinate of the lattice site and $j$ being the site index. The summation are on all the nearest-neighbor relations $\langle \alpha_j, \alpha'_j \rangle$. We consider two systems with the isotropic case for $t = t_1$ and the anisotropic one for $t \neq t_1$. The tunnelings between neighboring B and G sites are not considered and $t$ is taken as the unit of energy.

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$$H_{\text{dri}} = \sum_{\alpha_j} V(\alpha_j, t) \hat{n}_{\alpha_j}, \tag{2}$$

where $V(\alpha_j, t) = -\alpha_j \cdot \mathbf{F}(t)$ and $\hat{n}_{\alpha_j} = \hat{c}_{\alpha_j}^{\dagger} \hat{c}_{\alpha_j}$.
our analysis, the maximal strength of the shaking force is limited to twice of the frequency, i.e., $F_{\text{max}}a = 2\hbar\omega$ ($h = 1$). Therefore, it is reasonable to truncate the $\hat{H}_{\text{eff}}$ until $m = 2$ (see Fig. 2). Finally, the effective Hamiltonian is obtained as

$$\hat{H}_{\text{eff}} = \hat{H}_0 + \sum_{m=1,2} \left[ \hat{H}_m, \hat{H}_{-m} \right] + O(m \geq 3)$$

$$= \sum_{\langle R_j, B_j \rangle} t_{rb} \hat{c}_{R_j} \hat{c}_{B_j} + \sum_{\langle G_{j}, R_j \rangle} t_{gr} \hat{c}_{G_j} \hat{c}_{R_j} + \sum_{\langle R_j, R_j \rangle} t_{rr} \hat{c}_{R_j} \hat{c}_{R_j} + \sum_{\langle G_{j}, G_j \rangle} t_{bb} \hat{c}_{G_j} \hat{c}_{G_j} + h.c.,$$

where $\langle \cdots \rangle$ indicates the next-nearest-neighbor hoppings between the sublattice sites of the same type, and the hopping parameters are

$$t_{rb} = t_1 \mathcal{J}_0 (\beta),$$
$$t_{gr} = t_1 \mathcal{J}_0 (\beta),$$
$$t_{rr} = \frac{\sqrt{2}}{2}(\sqrt{t_{1}^{2} - t_{1}^{2}}) \mathcal{J}_1 (\beta) - \frac{1}{2} \mathcal{J}_2 (\beta),$$
$$t_{bb} = \frac{\sqrt{3} t_{1}^{2}}{2 \hbar \omega} e^{i\varphi} \left[ \mathcal{J}_1 (\beta) - \frac{1}{2} \mathcal{J}_2 (\beta) \right],$$
$$t_{gg} = \frac{3 t_{1}^{2}}{2 \hbar \omega} e^{i\varphi} \left[ \mathcal{J}_1 (\beta) - \frac{1}{2} \mathcal{J}_2 (\beta) \right],$$

where $\beta$ is the isotropic parameter satisfying $\beta = Fa/\hbar\omega$, and $\varphi = \pi/2$. $\mathcal{J}_{1,2,3}(\beta)$ is the $i$th-order Bessel function.

Having considered that the dice system preserves the translational symmetry, we can perform a SU(3) mapping [37] to transform the real-space $\hat{H}_{\text{eff}}$ into the quasi-momentum space. Based on the basis $(\hat{c}_{k,R}, \hat{c}_{k,B}, \hat{c}_{k,G})^T$ where $\hat{c}_{k,a} = \frac{1}{\sqrt{N}} \sum_{s} e^{-i\mathbf{k} \cdot \mathbf{r}_s} \hat{c}_{a,s}$ is the Fourier operation, the effective Bloch Hamiltonian is obtained as

$$\hat{H}_{\text{eff}} = \begin{pmatrix}
    d_3 + d_8 & d_1 - id_2 & d_4 - id_5 \\
    d_1 + id_2 & -d_3 + d_8 & 0 \\
    d_4 + id_5 & 0 & -2d_8
\end{pmatrix},$$

in which the matrix elements are

$$d_1 = t_{rb} \sum_{s} \cos (\mathbf{k} \cdot \mathbf{r}_s),$$
$$d_2 = t_{rb} \sum_{s} \sin (\mathbf{k} \cdot \mathbf{r}_s),$$
$$d_3 = -(|t_{gg}| + 2|t_{rr}|) \sum_{s} \sin (\mathbf{k} \cdot \delta_s),$$
$$d_4 = t_{gr} \sum_{s} \cos (\mathbf{k} \cdot \mathbf{r}_s),$$
$$d_5 = -t_{gr} \sum_{s} \sin (\mathbf{k} \cdot \mathbf{r}_s),$$
$$d_8 = |t_{gg}| \sum_{s} \sin (\mathbf{k} \cdot \delta_s),$$

where, the bond length has been set as $a = 1$, and the six vectors $\mathbf{r}_s$ and $\delta_s$ ($s = 1, 2, 3$) shown in Fig. 1(a) are

$$\mathbf{r}_1 = \begin{pmatrix} 0 \\ -1 \end{pmatrix}, \quad \mathbf{r}_2 = \frac{1}{2} \begin{pmatrix} \sqrt{3} \\ 1 \end{pmatrix}, \quad \mathbf{r}_3 = \frac{1}{2} \begin{pmatrix} -\sqrt{3} \\ 1 \end{pmatrix},$$

$$\delta_1 = \begin{pmatrix} \sqrt{3} \\ 0 \end{pmatrix}, \quad \delta_2 = \frac{1}{2} \begin{pmatrix} -\sqrt{3} \\ 3 \end{pmatrix}, \quad \delta_3 = \frac{1}{2} \begin{pmatrix} \sqrt{3} \\ 3 \end{pmatrix}.$$}

**IV. CHERN NUMBER AND EDGE STATE**

From the SU(3) mapping, we know that the effective Hamiltonian shows a three-level system. There are three quasi-energy bands denoted by $E_n(k)$ with $n = 1, 2, 3$. The increasing $n$ corresponds to the $n$-th quasi-energy band arranged in an ascending order. For the $n$-th band, its associated Chern number is [6, 33, 38–40]

$$C_n = \frac{1}{2\pi} \int_{FBZ} \Omega_n(k) d^2k,$$

where the integration extends over the first Brillouin zone (FBZ) and the $\Omega_n$ is the Berry curvature, which is defined in terms of the partial derivative of the eigenvector $|\psi_n(k)\rangle$ of $\hat{H}_{\text{eff}}(k)$ as $\Omega_n(k) = i \left( \frac{\partial \psi_n(k)}{\partial k_n} \frac{\partial \psi_n(k)}{\partial k_s} - h.c. \right).$
Here, we investigate the topological properties and the band structures of the driven dice system both in the isotropic and the anisotropic case. Without loss of generality, we choose \( t_1 = 0.5t \) to characterize the anisotropic case. By employing the definition of the Chern number in Eq. (11), the topological phase diagram that contains the Chern number of the lowest quasi-energy band \( C_1 \) as the function of \( \beta \) is plotted in Fig. 1, where the red dots correspond to the isotropic case and blue dots correspond to the anisotropic one. The Chern numbers of the middle band for the two cases are equal to zero, which are not shown in the phase diagram. Alternatively, the Chern numbers can be calculated by the analytical method (see the derivation in Appendix C), completely consistent with the numerical ones. Intuitively, without driving, namely \( \beta = 0 \), the system is topological trivial with \( C_1 = 0 \) and system keeps topological non-trivial once the driving is introduced. Differently, there are large Chern number \( C_1 = 2 \) for the isotropic case while \( C_1 = 1 \) for the anisotropic one. In fact, the Chern number of the static system is ill-defined because of the gapless dispersions of bands (see Figs. 3(b1) and 3(b2)). \( C_1 = 0 \) is used to conveniently characterize the trivial and gapless case. \( \Gamma \)-\( K \)-\( K' \)-\( \Gamma \) is the high-symmetry path where \( K \) and \( K' \) are the singularities [33, 40]. On the contrary, in the topological non-trivial phase, the bands are gapped. For instance, in the isotropic case, as shown in Figs. 3(c1) (\( \beta = 1 \)) and 3(d1) (\( \beta = 2 \)), three quasi-energy bands are separated by the gaps. Similar circumstance appears in the anisotropic case as well (\( \beta = 1 \) in Fig. 3(c2) and \( \beta = 2 \) in Fig. 3(d2)). Besides, we notice that there is difference between the two cases in the topological non-trivial phase. For the isotropic case, the middle quasi-energy band is fully a flat band (see Figs. 3(c1) and 3(d1)), but middle quasi-energy band is obviously distorted at the high-symmetry points \( K \) and \( K' \) in the anisotropic case.

Next, we select the isotropic case to discuss the correspondence between the Chern numbers and the edge modes according to the principle of the bulk-edge correspondence [36] in such a Floquet system. In fact, the anisotropic case supports this principle as well (see details in Appendix D). After choosing a cylindrical dice geometry which preserves the periodicity in the \( x \) direction but leaves it open in the \( y \) direction (armchair edge), the singly periodic Bloch Hamiltonian \( \mathcal{H}_{\text{eff}}(k_x) \) can be obtained by performing the partial Fourier transformation where \( k_x \) is the quantum number and \( k_x \in [-\pi/3, \pi/3] \). In the numerical calculation, we consider that the supercell contains total \( N_s = 297 \) lattice sites and take \( \beta = 1 \) and \( t_1 = t \). With these parameters, the singly periodic quasi-energy spectrum \( E(k_x) \) is plotted in Fig. 4(a). \( N_1, N_2, N_3, \) and \( N_4 \) are four chosen edge modes at \( E(k_x) \approx -0.075t \) (the dashed magenta line shows). \( M_1, M_2, M_3, \) and \( M_4 \) are another four edge modes chosen at \( E(k_x) \approx 0.075t \) (the dashed orange line shows). The spatial distributions of these edge modes are plotted in Figs. 4(b)-4(e). Particularly, the red curves character the modes with positive group velocity (PGV) while the black ones character the modes with negative group velocity (NGV). Intuitively, the modes with opposite quasi-momentum are symmetrically distributed at the edges of the dice geometry. Without loss of generality, we select the modes localized at the \( j = 1 \) side to analyze the bulk-edge correspondence. Since having known \( C_1 = 2 \), according the the modes \( N_2, N_4, M_1, \) and \( M_3 \) with PGV all carry the Chern number \( C = 1 \). As Ref. [36] tells, the Chern number of each band is the difference between the total Chern number carried by all the edge modes localized at one side above the band and the total Chern number carried by all the edge model localized at the same side below the band. Therefore, we extract the Chern number of the flat middle band \( C_2 \) as \( C_2 = 1 + 1 - (1 + 1) = 0 \), which is in accord with our results.

V. SUMMARY

In summary, the Floquet band engineering on the optical dice lattice has been well studied. Although the initially dice system possess gapless band structure, we uncover that the applied circular-frequency shaking will induce gapped quasi-energy bands and this non-trivial
band characteristic persists within a large strength of the shaking force. Furthermore, after investigating the topological properties of the isotropic case and the anisotropic case of the driven system, we find that in the isotropic case, there exists topological phase with Chern number \( C_1 = 2 \), higher than the one with \( C_1 = 1 \) in the anisotropic case. In the end, we discuss how to employ the associated edge modes to analyze the Chern number of quasi-energy bands within the framework of the principle of bulk-edge correspondence.

VI. ACKNOWLEDGMENTS

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Appendix A: Derivation of Equation (3)

The \( \hat{H}_{\text{rot}} \) in Eq. (3) can be expanded as

\[
\hat{H}_{\text{rot}} = \hat{U}^\dagger(t) \hat{H}_{\text{ini}} \hat{U}(t) = \sum_{\langle R_j, B_{j'} \rangle} t \left( \hat{U}^\dagger(t) \hat{c}_{R_j} \hat{U}(t) \hat{c}_{B_{j'}} + \text{H.c.} \right) + \sum_{\langle G_j, R_{j'} \rangle} t_1 \left( \hat{U}^\dagger(t) \hat{c}_{G_j} \hat{U}(t) \hat{c}_{R_{j'}} + \text{H.c.} \right),
\]

(A1)

where \( \hat{U}(t) = e^{\frac{i}{\hbar} \sum_{\alpha_j} \int_0^t [ - \alpha_j, \hat{F}(t) ] dt \cdot \hat{n}_{\alpha_j} } \). Employing the Baker-CAMPbell-Hausdorff formula [12, 34, 35],

\[
e^{i \hat{X} \hat{Y}} e^{-i \hat{X}} = \hat{Y} + i \hat{X}, \hat{Y} \hat{Y} - \frac{\hbar^2}{2!} \hat{X}, [\hat{X}, \hat{Y}] \hat{Y} + \frac{\hbar^3}{3!} \hat{X}, [\hat{X}, [\hat{X}, \hat{Y}]] \ldots,
\]

(A2)

we have

\[
\hat{U}^\dagger(t) \hat{c}_{\alpha_j} \hat{U}(t) = e^{\frac{i}{\hbar} \sum_{\alpha_j} \int_0^t \hat{F}(t) dt \cdot \hat{n}_{\alpha_j} } \hat{c}_{\alpha_j},
\]

(A3)

and

\[
\hat{U}^\dagger(t) \hat{c}_{\alpha_j} \hat{U}(t) = e^{\frac{i}{\hbar} \sum_{\alpha_j} \int_0^t \hat{F}(t) dt \cdot \hat{n}_{\alpha_j} } \hat{c}_{\alpha_j},
\]

(A4)

Therefore, the \( \hat{H}_{\text{rot}} \) is derived as

\[
\hat{H}_{\text{rot}} = \sum_{\langle R_j, B_{j'} \rangle} t \left( e^{-i \frac{\hbar}{2} \sin(\omega t + \theta^R_{B_{j'}})} \hat{c}_{R_j} \hat{c}_{B_{j'}} + \text{H.c.} \right) + \sum_{\langle G_j, R_{j'} \rangle} t_1 \left( e^{-i \frac{\hbar}{2} \sin(\omega t + \theta^G_{R_{j'}})} \hat{c}_{G_j} \hat{c}_{R_{j'}} + \text{H.c.} \right),
\]

(A5)

where \( \theta^{\alpha_j}_{\alpha_{j'}} \) is the direction angle from site \( \alpha_j \) to its neighbor \( \alpha_{j'} \),

Appendix B: Derivation of \( \hat{H}_m \)

The hopping strength in \( \hat{H}_{\text{rot}} \) can be rewritten as

\[
e^{-i \beta \sin(\omega t + \theta^R_{\alpha_{j'}})} = \exp \left[ \beta e^{-i(\omega t + \theta^R_{\alpha_{j'}})} - \frac{\hbar}{2} \right].
\]

(B1)

Employing the Jacobi-Anger expansion

\[
\exp \left[ \frac{\xi x - x^{-1}}{2} \right] = \sum_{\ell = -\infty}^{\infty} J_\ell(\xi) x^\ell,
\]

(B2)

\[
\hat{H}_{\text{rot}} \text{ is written as}
\]

\[
\hat{H}_{\text{rot}} = \sum_{\langle R_j, B_{j'} \rangle} t \left( \sum_{\ell = -\infty}^{\infty} J_\ell(\beta) e^{-i(\omega t + \theta^R_{B_{j'}})} \hat{c}_{R_j} \hat{c}_{B_{j'}} + \text{H.c.} \right) + \sum_{\langle G_j, R_{j'} \rangle} t_1 \left( \sum_{\ell = -\infty}^{\infty} J_\ell(\beta) e^{-i(\omega t + \theta^G_{R_{j'}})} \hat{c}_{G_j} \hat{c}_{R_{j'}} + \text{H.c.} \right).
\]

(B3)

Noticing that \( \hat{H}_{\text{rot}} \) is time-periodic, then it can be expanded as

\[
\hat{H}_{\text{rot}} = \sum_{m = -\infty}^{\infty} \hat{H}_m e^{im\omega t},
\]

(B4)

where \( \hat{H}_m \) is the \( m \)-th Fourier component of \( \hat{H}_{\text{rot}} \), from which we derive the \( \hat{H}_m \) as

\[
\hat{H}_m = \frac{\omega}{2\pi} \int_0^{2\pi} \hat{H}_{\text{rot}} e^{-im\omega t} dt
\]

\[
= \sum_{\langle R_j, B_{j'} \rangle} J \left( \sum_{m = -\infty}^{\infty} J_m(\beta) e^{im\theta^R_{B_{j'}}} \hat{c}_{R_j} \hat{c}_{B_{j'}} + \text{H.c.} \right)
\]

\[
+ \sum_{\langle G_j, R_{j'} \rangle} J_1 \left( \sum_{m = -\infty}^{\infty} J_m(\beta) e^{im\theta^G_{R_{j'}}} \hat{c}_{G_j} \hat{c}_{R_{j'}} + \text{H.c.} \right).
\]

(B5)
Appendix C: Derivation of the Chern number

We derive the analytical Chern number of the Hamiltonian presented in Eq. (8). In principle, all the eigenenergies and wavefunctions can be exactly solved, by which we can derive the Berry connection or the Berry curvature and then calculate the Chern number of each band after performing an integration [6]. However, the directly obtained eigenvalues and wavefunctions are rather complicated, and which are not convenient for us to derive the Berry connection or the Berry curvature directly. Therefore, we adopt an unconventional strategy to calculate the Chern number.

In the derivation, we suppose that each eigenvalue has clear expression in advance, but we do not know which band it belongs to. For a given eigenvalue \( \lambda_s(k) \) (\( s = 1, 2, 3 \)), its corresponding wavefunction \( |u_s(k)\rangle \) is given as

\begin{align*}
|u_s(k)\rangle &= \begin{pmatrix}
\frac{(\lambda_s(k)+d_3-d_8)(\lambda_s(k)+2d_8)}{\sqrt{(\lambda_s(k)+2d_8)^2(\lambda_s(k)+d_3-d_8)^2+(d_1^2+d_2^2)(\lambda_s(k)+2d_8)^2+(d_1^2+d_2^2)(\lambda_s(k)+d_3-d_8)^2}} \\
\frac{(d_1+id_2)(\lambda_s(k)+2d_8)}{\sqrt{(\lambda_s(k)+2d_8)^2(\lambda_s(k)+d_3-d_8)^2+(d_1^2+d_2^2)(\lambda_s(k)+2d_8)^2+(d_1^2+d_2^2)(\lambda_s(k)+d_3-d_8)^2}} \\
\frac{(d_1+id_2)(\lambda_s(k)+d_3-d_8)}{\sqrt{(\lambda_s(k)+2d_8)^2(\lambda_s(k)+d_3-d_8)^2+(d_1^2+d_2^2)(\lambda_s(k)+2d_8)^2+(d_1^2+d_2^2)(\lambda_s(k)+d_3-d_8)^2}}
\end{pmatrix}.
\end{align*}

(C1)

With \( |\psi_n(k)\rangle \), we derive the Berry connection as

\begin{align*}
\overrightarrow{A} &= -i \langle u_s(k)|\nabla_k|u_s(k)\rangle \\
&= \frac{(d_1 \nabla_k d_1 - d_2 \nabla_k d_1)(\lambda_s(k) + 2d_8)^2}{(\lambda_s(k) + 2d_8)^2(\lambda_s(k) + d_3 - d_8)^2 + (d_1^2 + d_2^2)(\lambda_s(k) + 2d_8)^2 + (d_1^2 + d_2^2)(\lambda_s(k) + d_3 - d_8)^2} \\
&\quad + \frac{(d_4 \nabla_k d_4 - d_5 \nabla_k d_4)(\lambda_s(k) + d_3 - d_8)^2}{(\lambda_s(k) + 2d_8)^2(\lambda_s(k) + d_3 - d_8)^2 + (d_1^2 + d_2^2)(\lambda_s(k) + 2d_8)^2 + (d_1^2 + d_2^2)(\lambda_s(k) + d_3 - d_8)^2}.
\end{align*}

(C2)

According to the generation of the TKNN theory in three-band system [33] and the one in the two-band system [40], we know that the Chern number of the band is contributed by the singularity \( q \), at which the Berry connection \( \overrightarrow{A} \) is singular. By analyzing the expression of \( \overrightarrow{A} \) in Eq. (C2), we extract that there are two types of singularities \( q^1 \) and \( q^2 \) in such a system. The first-type singularity \( q^1 \) makes

\begin{align*}
d_1 = d_2 = 0,
\end{align*}

(C3)

and contributes non-zero Chern numbers to the band with \( \lambda_s(k = q^1) = -d_3 + d_8 \). The second one \( q^2 \) makes

\begin{align*}
d_4 = d_5 = 0,
\end{align*}

(C4)

and contributes non-zero Chern numbers to the band with \( \lambda_s(k = q^2) = -2d_8 \).

We first discuss the first type case. In a concrete system, if there are more than one singularity satisfying the first-type of singularity condition, around the infinitesimal neighborhood of each first-type singularity \( q^1 \), the corresponding matrix elements can be expanded as

\begin{align*}
d_1^{q_1^1} &= a_{1x}^{q_1^1}\Delta k_x + a_{1y}^{q_1^1}\Delta k_y + O(\Delta k^2),
\end{align*}

(C5)

\begin{align*}
d_2^{q_1^1} &= a_{2x}^{q_1^1}\Delta k_x + a_{2y}^{q_1^1}\Delta k_y + O(\Delta k^2),
\end{align*}

Then, the Chern number contributed by \( q_1^1 \) is

\begin{align*}
C_{q_1^1} &= \frac{1}{2\pi} \oint_{q_1^1} \overrightarrow{A} q_1^1 \cdot dk \\
&= \text{sgn}(a_{1x}^{q_1^1}a_{2y}^{q_1^1} - a_{2x}^{q_1^1}a_{1y}^{q_1^1}).
\end{align*}

(C6)

For the second-type case, there may exist more than one singularity satisfying the singularity condition as well. Around the infinitesimal neighborhood of each second-type singularity \( q_2^1 \), the corresponding \( d_1^{q_2^1} \) and \( d_2^{q_2^1} \) can be expanded as the similar form

\begin{align*}
d_1^{q_2^1} &= a_{4x}^{q_2^1}\Delta k_x + a_{4y}^{q_2^1}\Delta k_y + O(\Delta k^2),
\end{align*}

(C7)

\begin{align*}
d_2^{q_2^1} &= a_{5x}^{q_2^1}\Delta k_x + a_{5y}^{q_2^1}\Delta k_y + O(\Delta k^2).
\end{align*}

(C7)
Then, the Chern number contributed by $\mathbf{q}_j^1$ is

$$C_{\mathbf{q}_j^1} = \frac{1}{2\pi i} \int_{\mathbf{q}_j^1} \mathbf{A}_{\mathbf{q}_j^1} \cdot d\mathbf{k} = \text{sgn}(a_{d_x}^2 a_{d_y}^2 - a_{d_z}^2 a_{d_y}^2).$$  \hspace{1cm} \text{(C8)}

Up to now, we have known the types of singularities in this generalized system and the expressions of the Chern numbers they contribute. Moreover, from their expressions, we know that $C_{\mathbf{q}_j^1}$ and $C_{\mathbf{q}_j^2}$ only depend on the expansion coefficients while have nothing to with whether the system is in the isotropic case or in the anisotropic one. Nevertheless, two key problems remain to be solved. The first one is that which bands $\lambda_1(\mathbf{q}_j^1)$ and $\lambda_2(\mathbf{q}_j^1)$ correspond to. The second one is the sum of Chern numbers contributed by the two kinds of singularities to each band. To answer the questions, it is necessary to analyze the eigenenergies at the singularities. Around the first-type singularity $\mathbf{q}_j^1$, the Hamiltonian can be reexpressed as

$$\hat{H}_{\text{eff}}^{\mathbf{q}_j^1} = \hat{H}_0(\mathbf{k} = \mathbf{q}_j^1) + \hat{H}'_{\mathbf{q}_j^1}$$

$$= \begin{pmatrix}
    d_3 + d_4 & 0 & d_1 - id_5 \\
    0 & -d_3 + d_8 & 0 \\
    d_4 + id_5 & 0 & -2d_8 \\
\end{pmatrix}$$

$$+ \begin{pmatrix}
    d_1^0 & -id_2^0 & 0 \\
    0 & d_2^0 & 0 \\
    0 & 0 & 0 \\
\end{pmatrix},$$  \hspace{1cm} \text{(C9)}

where $\hat{H}'_{\mathbf{q}_j^1}$ is regarded as the perturbation term. Under the second-order perturbation approximation, the eigenenergies around $\mathbf{q}_j^1$ are

$$\lambda_1(\mathbf{q}_j^1) = -d_3 + d_4,$n

$$\lambda_2(\mathbf{q}_j^1) = -d_3 + d_8 - \sqrt{(d_3 + 3d_8)^2 + d_2^2 + d_5^2},$$

$$\lambda_3(\mathbf{q}_j^1) = -d_3 + d_8 + \sqrt{(d_3 + 3d_8)^2 + d_2^2 + d_5^2}. \hspace{1cm} \text{(C10)}$$

We can determine the Chern number of the three bands just by comparing $\lambda_1(\mathbf{q}_j^1)$ with $\lambda_2(\mathbf{q}_j^1)$ and $\lambda_3(\mathbf{q}_j^1)$. For instance, if $\lambda_1(\mathbf{q}_j^1)$ is the smallest one among the three eigenenergies, i.e., $\lambda_1(\mathbf{q}_j^1) \equiv E_1(\mathbf{q}_j^1)$, then the lowest band $E_1$ has the non-zero Chern number $C_{\mathbf{q}_j^1}$, while the Chern number of other two bands are both equal to zero.

In the same way, we reexpress the Hamiltonian around the second-type singularity $\mathbf{q}_j^2$ as

$$\hat{H}_{\text{eff}}^{\mathbf{q}_j^2} = \hat{H}_0(\mathbf{k} = \mathbf{q}_j^2) + \hat{H}'_{\mathbf{q}_j^2}$$

$$= \begin{pmatrix}
    d_3 + d_8 & d_1 - id_2 & 0 \\
    d_1 + id_2 & -d_3 + d_8 & 0 \\
    0 & 0 & -2d_8 \\
\end{pmatrix}$$

$$+ \begin{pmatrix}
    0 & 0 & 0 \\
    0 & 0 & 0 \\
    d_4^2 & id_5^2 & 0 \\
\end{pmatrix},$$  \hspace{1cm} \text{(C11)}

where $\hat{H}'_{\mathbf{q}_j^2}$ is regarded as the perturbation term. Under the second-order perturbation approximation, the eigenenergies around $\mathbf{q}_j^2$ are

$$\lambda_1(\mathbf{q}_j^2) = -2d_8,$

$$\lambda_2(\mathbf{q}_j^2) = d_5 - \sqrt{d_1^2 + d_2^2 + d_5^2},$$

$$\lambda_3(\mathbf{q}_j^2) = d_5 + \sqrt{d_1^2 + d_2^2 + d_5^2}. \hspace{1cm} \text{(C12)}$$

Following the same analysis method as the first-type case, by comparing $\lambda_1(\mathbf{q}_j^2)$ with $\lambda_2(\mathbf{q}_j^2)$ and $\lambda_3(\mathbf{q}_j^2)$, we can determine which band the $\lambda_1(\mathbf{q}_j^2)$ corresponds to. If $\lambda_1(\mathbf{q}_j^2)$ is the largest one among the three eigenenergies, then the highest band $E_3$ has a non-zero Chern number $C_{\mathbf{q}_j^2}$. Otherwise, the middle band $E_2$ or the lowest band $E_1$ has a non-zero Chern number $C_{\mathbf{q}_j^2}$. Based on the above analysis, we conclude that the Chern number of a concrete band is the summation of the Chern numbers contributed by all singularities to the band.

In the following, we choose the isotropic case with $t_1 = t$ and $\beta = 1$ and the anisotropic case with $t_1 = \frac{t}{2}$ and $\beta = 2$ as two examples, and then calculate the Chern numbers of the two examples by this analytical method. After comparing the four matrix elements $d_1$, $d_2$, $d_4$, and $d_5$ in Eq. \((9)\), we find that the singularities satisfying the first-type singularity condition satisfy the second-type singularity condition as well. To obtain the Chern number of the special case, we just have to substitute the expansion coefficients of the four matrix elements into the definitions of the first-type Chern number and the second-type one, respectively. Then we calculate the Chern number of each band according to the above mentioned summation rule.

From the singularity condition, we extract two singularities simultaneously satisfying the first-type and second-type condition. One is $\mathbf{q}_j^1 \left( \mathbf{q}_j^2 \right) = K \equiv \left( \frac{4\pi}{3\sqrt{3}}, 0 \right)$ and the other is $\mathbf{q}_j^2 \left( \mathbf{q}_j^2 \right) = K' \equiv \left( \frac{2\pi}{3\sqrt{3}}, \frac{2\pi}{3} \right)$. For the
first-type singularity case, the expansion coefficients are
\[ a_{11}^q = -\frac{3}{2}t_{rb}, \quad a_{21}^q = 0, \]
\[ a_{22}^q = 0, \quad a_{42}^q = -\frac{3}{2}t_{rb}, \]  
\[ a_{12}^q = -\frac{3}{4}t_{rb}, \quad a_{22}^q = -\frac{3\sqrt{3}}{4}t_{rb}, \]
\[ a_{42}^q = -\frac{3\sqrt{3}}{4}t_{rb}, \quad a_{22}^q = -\frac{3}{4}t_{rb}. \]  
\[ (C13) \]

From Fig. 2, we know that the parameter \( t_{rb} \) and \( t_{gr} \) are indeed positive numbers either in the isotropic case or in the anisotropic case. Substituting these expansion coefficients into the definition of \( C_{q_j^1} \) in Eq. (6), we have
\[ C_{q_j^1} = 1, \quad C_{q_j^2} = -1. \]  
\[ (C14) \]

For the second-type singularity case, the expansion coefficients are
\[ a_{11}^q = -\frac{3}{2}t_{gr}, \quad a_{21}^q = 0, \]
\[ a_{22}^q = 0, \quad a_{42}^q = \frac{3}{2}t_{gr}, \]
\[ a_{12}^q = -\frac{3}{4}t_{gr}, \quad a_{22}^q = -\frac{3\sqrt{3}}{4}t_{gr}, \]
\[ a_{42}^q = -\frac{3\sqrt{3}}{4}t_{gr}, \quad a_{22}^q = -\frac{3}{4}t_{gr}. \]  
\[ (C15) \]

Substituting the expansion coefficients into the definition of \( C_{q_j^2} \) in Eq. (8), we have
\[ C_{q_j^2} = -1, \quad C_{q_j^2} = 1. \]  
\[ (C16) \]

Next, we analyze that which band \( C_{q_j^1} \) or \( C_{q_j^2} \) corresponds to. At \( q_j^1 \), the eigenenergies are
\[ \lambda_1(q_j^1) = \sum_{s=1,2,3} 2|t_{hh}| \sin (k \cdot q_j^1), \]
\[ \lambda_2(q_j^1) = \sum_{s=1,2,3} -2|t_{rr}| \sin (k \cdot q_j^1), \]
\[ \lambda_3(q_j^1) = \sum_{s=1,2,3} -2|t_{gg}| \sin (k \cdot q_j^1). \]  
\[ (C17) \]

After comparing the three eigenenergies, we find that \( C_{q_j^1} = 1 \) corresponds to the lowest band \( E_1 \) and \( C_{q_j^2} = 1 \) corresponds to the highest band \( E_3 \) both in the isotropic and anisotropic cases.

At \( q_j^2 \), the eigenenergies are
\[ \lambda_1(q_j^2) = \sum_{s=1,2,3} -2|t_{gg}| \sin (k \cdot q_j^2), \]
\[ \lambda_2(q_j^2) = \sum_{s=1,2,3} 2|t_{hh}| \sin (k \cdot q_j^2), \]
\[ \lambda_3(q_j^2) = \sum_{s=1,2,3} -2|t_{rr}| \sin (k \cdot q_j^2). \]  
\[ (C18) \]

Similarly, by comparing the three eigenenergies, we find that in the isotropic case, \( C_{q_j^2} = -1 \) corresponds to the highest band \( E_3 \) and \( C_{q_j^2} = 1 \) corresponds to the lowest band \( E_1 \), whereas in the anisotropic case, both \( C_{q_j^2} = -1 \) and \( C_{q_j^2} = 1 \) correspond to the middle band \( E_2 \). Synthesizing the above analysis, we have: In the isotropic case, the Chern numbers are \( C_1 = 1 + 1 = 2, \quad C_2 = 0, \) and \( C_3 = -2, \) respectively; in the anisotropic case, the Chern numbers are \( C_1 = 1, \quad C_2 = 0, \) and \( C_3 = -1, \) respectively.

![Figure 5](image_url)

Figure 5. (Color Online) (a) Singly periodic quasi-energy spectrum \( E(k_x) \) as a function of the quasi-momentum \( k_x \) in the anisotropic case. \( Q_1 \) and \( Q_2 \) are a pair of edge modes chosen at \( E(k_x) \approx -0.075t \) (the magenta dashed line). \( P_1 \) and \( P_2 \) are another pair of edge modes chosen at \( E(k_x) \approx 0.075t \) (the orange dashed line). Panels (b) and (c) present spatial distributions of these chosen edge modes. The modes with opposite quasi-momentum are symmetrically distributed at the edges of the dice geometry.

Appendix D: The bulk-edge correspondence in anisotropic case

Still considering the armchair dice geometry and taking \( N_s = 297 \), the singly periodic quasi-energy spectrum \( E(k_x) \) of the anisotropic case is plotted in Fig. 5(a). \( Q_1 \) and \( Q_2 \) are a pair of edge mode with opposite quasi-momentum \( k_x \) chosen at \( E(k_x) \approx -0.1 \). \( P_1 \) and \( P_2 \) are another pair of edge modes with opposite \( K_x \) chosen at \( E(k_x) \approx 0.1 \). Figures 5(b) and 5(c) present the spatial distributions of these chosen edge modes. It is readily seen that the modes with opposite quasi-momentum are symmetrically distributed at the edges of the dice geometry. We analyze the bulk-edge correspondence by selecting the modes localized at the \( N_s = 297 \) side. As discussed in the isotropic case, the modes \( Q_1 \) and \( P_2 \) with PGV both correspond to the Chern number \( C = 1 \). Therefore, we know that the Chern number of the lowest
quasi-energy band $C_1$ is $C_1 = 1$ and the Chern number of the middle quasi-energy band $C_2$ is $C_2 = 1 - 1 = 0$, which are the same as the numerical and analytical results.

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