SU(3) Spin-Orbit Coupling in Systems of Ultracold Atoms

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Motivated by the recent experimental success in realizing synthetic spin-orbit coupling in ultracold atomic systems, we consider N-component atoms coupled to a non-Abelian $SU(N)$ gauge field. More specifically, we focus on the case, referred to here as "SU(3) spin-orbit-coupling," where the internal states of three-component atoms are coupled to their momenta via a matrix structure that involves the Gell-Mann matrices (in contrast to the Pauli matrices in conventional SU(2) spin-orbit-coupled systems). It is shown that the SU(3) spin-orbit-coupling gives rise to qualitatively different phenomena and in particular we find that even a homogeneous SU(3) field on a simple square lattice enables a topologically nontrivial state to exist, while such SU(2) systems always have trivial topology. In deriving this result, we first establish an equivalence between the Hofstadter model with a $1/N$ Abelian flux per plaquette and a homogeneous $SU(N)$ non-Abelian model. The former is known to have a topological spectrum for $N > 2$, which is thus inherited by the latter. It is explicitly verified by an exact calculation for $N = 3$, where we develop and use a new algebraic method to calculate topological indices in the SU(3) case. Finally, we consider a strip geometry and establish the existence of three gapless edge states—the hallmark feature of such an SU(3) topological insulator.

PACS numbers: 67.85.−d, 03.75.−b, 37.10.Gh, 71.70.Ej

Following the theoretical prediction [1,2] and experimental observation [3] of the quantum spin hall effect, topological states of matter have received a recent surge of attention. The classification of topological states of matter lies outside of the Landau symmetry breaking paradigm, and is instead determined by topological quantum numbers [4]. The existence of nonzero topological numbers often has important physical consequences for finite systems, including the existence of edge states [5]. Strong spin-orbit coupling is central to the experimental realization of the quantum spin hall effect. Spin-orbit coupling has a long history in solid-state systems and can play a number of important roles [6]. Recently, interest in spin-orbit coupling has come to the fore in the seemingly disparate area of ultracold atoms with the advent of synthetic gauge fields [7]. Such gauge fields have been employed to mimic magnetic fields [8–11] as well as Rashba-Dresselhaus spin-orbit coupling in both bosons [12] and fermions [13]. This progress opens doors not only to quantum simulation of spin-orbit coupled solid-state systems [14,15], but also to the realization of a much larger class of structures that can be engineered in the ultracold laboratory but do not exist in the solid state (see, for instance, Refs. [16–18]).

In this Letter, motivated by the recent advances in ultracold atoms, we introduce the notion of $SU(N)$ spin-orbit coupling. In particular, we consider a system of atoms in a square optical lattice under the presence of spin-orbit coupling corresponding to a spatially homogeneous gauge field, as such gauge fields are experimentally simpler to realize [16]. We show that for $N = 2$ (the case most relevant in the solid state) all such Hamiltonians are topologically trivial. On the other hand for $N = 3$ (as can be realized with ultracold atoms with internal spin degrees of freedom [19] but which is less relevant for solid state systems), by direct construction we show that such systems with nontrivial topological numbers exist. This topological property results in the physically interesting situation of gapless edge modes, while the bulk spectrum remains gapped. Such modes can be experimentally probed through *in situ* imaging [20], time-of-flight spectroscopy [21], or Bragg spectroscopy [22]. The experimental realization of the fairly simple resulting three-component Hamiltonian would pave the way to the realization of topological states of matter in the ultracold laboratory.

The conventional spin-orbit coupling in solid state systems manifests itself as a Zeeman magnetic field that depends on the electron's momentum [6]. Hence a typical spin-orbit term in a continuum model of a solid is $\mathbf{b}(\mathbf{p}) \cdot \hat{\boldsymbol{\sigma}}$, where the form of the momentum-dependent internal field, $\mathbf{b}(\mathbf{p})$, is dictated by symmetries of the crystal structure and $\hat{\boldsymbol{\sigma}}$ is a vector of Pauli matrices, which mathematically are generators of the SU(2) group that act on the electron's SU(2) spin. In contrast to solids, synthetic spin-orbit structures in ultracold atoms are built from the ground up and are not constrained by fundamental symmetries. Furthermore, since the "spin" itself is synthetic, there is no requirement that it be associated with a representation of the SU(2) group. Hence, a much larger space of $SU(N)$ spin-orbit couplings becomes available for multicomponent atoms, $\sum_i b^i(\mathbf{p}) \hat{X}_i$, where $\hat{X}_i$ are in principle any of the $(N^2 - 1)$

Hermitian generators of SU(N) (e.g., the Pauli matrices for $N = 2$, the Gell-Mann matrices for $N = 3$, etc.).

The Bloch Hamiltonian for a square lattice with nearest neighbor hopping under the presence of a homogeneous SU(N) gauge field is given by

$$\hat{\mathcal{H}}(\mathbf{k}) = -2t[\cos(k_x - \hat{A}_x) + \cos(k_y - \hat{A}_y)], \quad (1)$$

where t is the hopping and the gauge fields $\hat{A}_{x,y}$ are constant $N \times N$ Hermitian matrices. To make the connection with spin-orbit coupling clear, the cosines can be expanded and the Bloch Hamiltonian can be rewritten as $\hat{\mathcal{H}}(\mathbf{k}) = a(\mathbf{k}) + \sum_i b^i(\mathbf{k})\hat{X}_i$. To construct an "SU(3) topological insulator" we relate the model of Eq. (1) to the Hofstadter model [23], familiar from quantum Hall physics, which describes particles hopping on a square lattice under a uniform magnetic field (but nonuniform gauge field). To extend the Hofstadter model to SU(N) systems we consider N decoupled replicas, each having the same flux per plaquette. Our starting point is thus the Hamiltonian

$$H_{\mathrm{HM}} = -t\sum_i (\Psi_i^\dagger \Psi_{i+\hat{\mathbf{x}}} + \Psi_i^\dagger e^{-i2\pi\alpha(x_i + \hat{S}_z)}\Psi_{i+\hat{\mathbf{y}}} + \mathrm{H.c.}).$$
$$(2)$$

In this equation $\Psi_i = (\psi_{i1}, \psi_{i2}, \ldots, \psi_{iN})^T$ are SU(N) spinor operators, $\hat{S}_z = \mathrm{diag}(s, s-1, \ldots, -s)$ where $2s + 1 = N$, $\hat{\mathbf{x}}$ and $\hat{\mathbf{y}}$ are the two square lattice vectors where the lattice constant is set to unity, $x_i = \hat{\mathbf{x}} \cdot \mathbf{r}_i$ where $\mathbf{r}_i$ is the position of the ith lattice site, and α gives the magnitude of the flux. Since $\hat{S}_z$ is diagonal in this representation, the model trivially decouples into N independent copies of the Hofstadter model, each having $2\pi\alpha$ flux per plaquette. We restrict the flux to be related to the number of spin components as $\alpha = 1/N$.

We will first illustrate the mapping for the case of two-component spins and later describe how to generalize. For this case we apply the gauge transformation $\Psi_i \rightarrow e^{-i(\pi/2)\hat{\sigma}_x x_i}\Psi_i$ where $\hat{\sigma}_x$ is a Pauli matrix. This transformation rotates the spinors about the x axis by a position-dependent angle. As can be seen after some straightforward algebra, this transformation removes the spatial dependence of the second term in Eq. (2) at the cost of introducing a non-Abelian x-component into the gauge field. In particular, after the gauge transformation Eq. (2) becomes

$$H = -t\sum_i (\Psi_i^\dagger e^{-i\hat{A}_x}\Psi_{i+\hat{\mathbf{x}}} + \Psi_i^\dagger e^{-i\hat{A}_y}\Psi_{i+\hat{\mathbf{y}}} + \mathrm{H.c.})$$
$$= \sum_{\mathbf{k}} \Psi_{\mathbf{k}}^\dagger \hat{\mathcal{H}}(\mathbf{k})\Psi_{\mathbf{k}}, \quad (3)$$

where in the second line we have taken the Fourier transform. For this case, the non-Abelian gauge fields of Eq. (1) can be expressed as Pauli matrices as $(\hat{A}_x, \hat{A}_y) = \frac{\pi}{2}(\hat{\sigma}_x, \hat{\sigma}_z)$. The Bloch Hamiltonian can also be expanded

and rewritten as $\hat{\mathcal{H}}(\mathbf{k}) = -2t[\sin(k_x)\hat{\sigma}_x + \sin(k_y)\hat{\sigma}_z]$ which is a lattice version of Rashba spin-orbit coupling.

We now generalize this mapping to any integer N. As before, we perform a gauge transformation $\Psi_i \rightarrow \hat{\mathcal{U}}^{x_i}\Psi_i$. The unitary matrix $\hat{\mathcal{U}}$ is defined to have $\hat{\mathcal{U}}_{1,N} = \hat{\mathcal{U}}_{n+1,n} = -i$ for $1 \le n \le N - 1$ with zeroes elsewhere. One can verify for this matrix that $\hat{\mathcal{U}}^\dagger e^{-i2\pi\alpha\hat{S}_z}\hat{\mathcal{U}} = e^{-i2\pi\alpha(\hat{S}_z - 1)}$. Therefore this gauge transformation will completely remove the position dependence of the second term in Eq. (2), and the transformed Hamiltonian will correspond to particles on a square lattice under a homogeneous gauge field.

The SU(3) case of this general mapping will be considered in detail below. For this case, the non-Abelian gauge fields arrived at through the mapping which enters Eq. (1) can be expressed in terms of Gell-Mann matrices [24] as

$$\hat{A}_x = \frac{2\pi}{3\sqrt{3}}(\hat{\lambda}_2 - \hat{\lambda}_5 + \hat{\lambda}_7) \quad \text{and} \quad \hat{A}_y = \frac{\pi}{3}(\hat{\lambda}_3 + \sqrt{3}\hat{\lambda}_8).$$
$$(4)$$

By expanding the cosines, the Bloch Hamiltonian can also be written as $\hat{\mathcal{H}}(\mathbf{k}) = \mathbf{b}(\mathbf{k}) \cdot \hat{\boldsymbol{\lambda}}$ where $\mathbf{b}(\mathbf{k}) = -t(\cos(k_x), \sin(k_x), \frac{\sqrt{3}}{2}\sin(k_y) - \frac{3}{2}\cos(k_y), \cos(k_x), -\sin(k_x), \cos(k_x), \sin(k_x), \frac{\sqrt{3}}{2}\cos(k_y) + \frac{3}{2}\sin(k_y))$ is an eight-component vector and $\hat{\boldsymbol{\lambda}}$ is a vector composed of the eight Gell-Mann 3×3 matrices.

Geometrical method for Berry curvature and Chern number computation.—We now describe a geometrical method of computing the Berry curvature and Chern numbers for general SU(3) systems. We first write down expressions which are valid for any N. The Berry curvature $\Omega n(\mathbf{k})$ [25] is defined in terms of the normalized eigenstates $\chi_{\mathbf{k}n}$ of the Bloch Hamiltonian as

$$\Omega_n(\mathbf{k}) = i(\partial_{k_x}\chi_{\mathbf{k}n}^\dagger \partial_{k_y}\chi_{\mathbf{k}n} - \partial_{k_y}\chi_{\mathbf{k}n}^\dagger \partial_{k_x}\chi_{\mathbf{k}n}), \quad (5)$$

where n labels the eigenstate (or band). The Chern number for a particular band is defined as [26]

$$\nu_n = \frac{1}{2\pi}\int_{\mathrm{BZ}} d^2k\, \Omega_n(\mathbf{k}), \quad (6)$$

where the integral is performed over the first Brillouin zone (BZ). The Berry curvature can also be expressed in terms of eigenstate projection operators $\hat{P}_{\mathbf{k}n} = \chi_{\mathbf{k}n} \otimes \chi_{\mathbf{k}n}^\dagger$, where $\otimes$ denotes the outer product, through the useful relation [27,28]

$$\Omega_n(\mathbf{k})dk_x \wedge dk_y = i\mathrm{Tr}(\hat{P}_{\mathbf{k}n} \wedge d\hat{P}_{\mathbf{k}n} \wedge d\hat{P}_{\mathbf{k}n}), \quad (7)$$

where $dk_x \wedge dk_y = -dk_y \wedge dk_x$.

Before generalizing we first describe a well-known geometrical expression for the Berry curvature for SU(2) systems (see, e.g., Ref. [29]). This will be used to demonstrate that SU(2) Bloch Hamiltonians of the form of Eq. (1) are in general topologically trivial. The Bloch Hamiltonian

for SU(2) systems can be expressed in terms of Pauli matrices as $\hat{\mathcal{H}}(\mathbf{k}) = a(\mathbf{k}) + \mathbf{b}(\mathbf{k}) \cdot \hat{\boldsymbol{\sigma}}$. The projection operators corresponding to the two eigenstates can be written in terms of $\mathbf{b}(\mathbf{k})$ as $\hat{P}_{\mathbf{k}\pm} = \frac{1}{2}[1 \pm \mathbf{b}(\mathbf{k}) \cdot \hat{\boldsymbol{\sigma}}/|\mathbf{b}(\mathbf{k})|]$. Inserting this into Eq. (7) then gives

$$\Omega_{\pm}(\mathbf{k}) = \mp \frac{1}{2|\mathbf{b}(\mathbf{k})|^3} \mathbf{b}(\mathbf{k}) \cdot [\partial_{k_x} \mathbf{b}(\mathbf{k}) \times \partial_{k_y} \mathbf{b}(\mathbf{k})]. \quad (8)$$

Thus, the Berry curvature can be expressed directly in terms of the Bloch Hamiltonian, rendering the intermediate steps of computing its eigenstates and evaluating Eq. (5) unnecessary. For SU(2) systems, one can write arbitrary gauge fields of $\hat{\mathcal{H}}(\mathbf{k})$ as linear combinations of Pauli matrices as $\hat{A}_{x,y} = u_{x,y} + \mathbf{v}_{x,y} \cdot \hat{\boldsymbol{\sigma}}$. After expanding the exponents to obtain $\mathbf{b}(\mathbf{k})$, it is a straightforward exercise to verify that $\partial_{k_x}\mathbf{b}(\mathbf{k}) \times \partial_{k_y}\mathbf{b}(\mathbf{k}) \propto \mathbf{v}_x \times \mathbf{v}_y$. Then through Eq. (8) one sees that the Berry curvature vanishes identically, rendering SU(2) systems described by Eq. (1) topologically trivial.

We now move on to develop a central technical result of our work, namely the generalization of Eq. (8) to SU(3) systems. We will utilize the elegant formalism presented in Ref. [30] which describes an efficient way to represent pure-state density matrices (or projection operators) for three-state systems. For SU(3) systems, a general Bloch Hamiltonian can be expressed in terms of the eight Gell-Mann matrices as

$$\hat{\mathcal{H}}(\mathbf{k}) = a(\mathbf{k}) + \mathbf{b}(\mathbf{k}) \cdot \hat{\boldsymbol{\lambda}}, \quad (9)$$

where $a(\mathbf{k})$ is a scalar and $\mathbf{b}(\mathbf{k})$ is an eight-dimensional real vector. The product of two Gell-Mann matrices can be written as $\hat{\lambda}_a \hat{\lambda}_b = \frac{2}{3}\delta_{ab} + d_{abc}\hat{\lambda}_c + if_{abc}\hat{\lambda}_c$ where d_{abc} and f_{abc} are the symmetric and antisymmetric structure constants of SU(3) [24]. These structure constants define three bilinear operations for the eight-component vectors. In particular, one has the dot product $\mathbf{u} \cdot \mathbf{v} = u_a v_a$, the cross product $(\mathbf{u} \times \mathbf{v})_a = f_{abc}u_b v_c$, and the so-called star product [30] $(\mathbf{u} * \mathbf{v})_a = \sqrt{3}d_{abc}u_b v_c$ for two arbitrary vectors $\mathbf{u}$ and $\mathbf{v}$ where repeated indices are summed over. One can also write eigenstate projection operators in terms of the Gell-Mann matrices as

$$\hat{P}_{\mathbf{k}n} = \chi_{\mathbf{k}n} \otimes \chi_{\mathbf{k}n}^{\dagger} = \frac{1}{3}(1 + \sqrt{3}\mathbf{n}_{\mathbf{k}n} \cdot \hat{\boldsymbol{\lambda}}), \quad (10)$$

where $\text{Tr}\hat{P}_{\mathbf{k}n} = 1$. The condition that $(\hat{P}_{\mathbf{k}n})^2 = \hat{P}_{\mathbf{k}n}$, leads to two constraints on the vector $\mathbf{n}_{\mathbf{k}n}$ which are $\mathbf{n}_{\mathbf{k}n} \cdot \mathbf{n}_{\mathbf{k}n} = 1$ and $\mathbf{n}_{\mathbf{k}n} * \mathbf{n}_{\mathbf{k}n} = \mathbf{n}_{\mathbf{k}n}$ [30]. Due to the star-product constraint, $\mathbf{n}_{\mathbf{k}n}$ lies in a restricted region of S^7. This can be compared to the SU(2) system where the vector analogous to $\mathbf{n}_{\mathbf{k}n}$ can lie anywhere in S^2.

Now we will express $\mathbf{n}_{\mathbf{k}n}$ in terms of $\mathbf{b}(\mathbf{k})$ appearing in the Bloch Hamiltonian of Eq. (9). For projection operators corresponding to eigenstates we have $[\hat{P}_{\mathbf{k}n}, \hat{\mathcal{H}}(\mathbf{k})] = 0$ so that $\mathbf{b}(\mathbf{k}) \times \mathbf{n}_{\mathbf{k}n} = 0$. One can verify that this equation,

along with the above constraints, is satisfied by $\mathbf{n}_{\mathbf{k}n} = \xi_{\mathbf{k}n}[\gamma_{\mathbf{k}n}\mathbf{b}(\mathbf{k}) + \mathbf{b}(\mathbf{k}) * \mathbf{b}(\mathbf{k})]$ with coefficients

$$\gamma_{\mathbf{k}n} = 2|\mathbf{b}(\mathbf{k})| \cos\left(\theta_{\mathbf{k}} + \frac{2\pi}{3}n\right),$$
$$\xi_{\mathbf{k}n} = \frac{1}{|\mathbf{b}(\mathbf{k})|^2[4\cos^2(\theta_{\mathbf{k}} + \frac{2\pi}{3}n) - 1]}, \quad (11)$$

where $\theta_{\mathbf{k}} = \frac{1}{3}\arccos[\frac{\mathbf{b}(\mathbf{k}) \cdot \mathbf{b}(\mathbf{k}) * \mathbf{b}(\mathbf{k})}{|\mathbf{b}(\mathbf{k})|^3}]$ and n runs from one to three. The resulting expression for $\hat{P}_{\mathbf{k}n}$ can be inserted into Eq. (7) to obtain the Berry curvature. One finds

$$\Omega_n(\mathbf{k}) = -\frac{4\xi^3}{3^{3/2}}[\gamma^2 \partial_{k_x}\mathbf{b} \times \partial_{k_y}\mathbf{b} + \gamma \partial_{k_x}\mathbf{b} \times \partial_{k_y}(\mathbf{b} * \mathbf{b})$$
$$+ \gamma \partial_{k_x}(\mathbf{b} * \mathbf{b}) \times \partial_{k_y}\mathbf{b} + \partial_{k_x}(\mathbf{b} * \mathbf{b})$$
$$\times \partial_{k_y}(\mathbf{b} * \mathbf{b})] \cdot (\gamma\mathbf{b} + \mathbf{b} * \mathbf{b}), \quad (12)$$

where we have suppressed the $\mathbf{k}$, n arguments on the right-hand side. Notice that due to orthogonality relations, the derivatives do not act on the coefficients. While Eq. (12) is complicated in appearance, it is straightforward to compute with a given $\mathbf{b}(\mathbf{k})$. This equation provides an explicit expression for the Berry curvature in terms of quantities from the Bloch Hamiltonian and thus should be viewed as a generalization of Eq. (8) to SU(3) systems.

Analysis of SU(3) model.—Having established the above formalism, we now move on to analyze the specific SU(3) model arrived at above, given by Eqs. (1) and (4). The resulting $\mathbf{b}(\mathbf{k})$ can be directly inserted into Eqs. (11) and (12) to find the Berry curvature for this system. One finds

$$\Omega_n(\mathbf{k}) = \frac{2\cos(4\theta_{\mathbf{k}} + \frac{2\pi}{3}n) - 3}{\sqrt{3}[1 + 2\cos(2\theta_{\mathbf{k}} - \frac{2\pi}{3}n)]^3}, \quad (13)$$

where $\theta_{\mathbf{k}} = \frac{1}{3}\arccos[\frac{-1}{\sqrt{8}}(\cos(3k_x) + \cos(3k_y))]$. In addition, using the expression $E_{\mathbf{k}n} = \text{Tr}\{\hat{P}_{\mathbf{k}n}\hat{\mathcal{H}}(\mathbf{k})\}$, the bulk eigenenergies are found to be

$$E_{\mathbf{k}n} = 2\sqrt{2}t \frac{\cos(3\theta_{\mathbf{k}}) + 2\cos(\theta_{\mathbf{k}} + \frac{2\pi}{3}n)}{1 + 2\cos(2\theta_{\mathbf{k}} + \frac{2\pi}{3}n)}. \quad (14)$$

These bands are gapped and ordered such that $E_{\mathbf{k}1} < E_{\mathbf{k}2} < E_{\mathbf{k}3}$. With the above expressions for the curvature, the Chern numbers can be computed via Eq. (6) and are found to be $(\nu_1, \nu_2, \nu_3) = (-3, 6, -3)$.

Due to the bulk-boundary correspondence [5], nonzero Chern numbers imply the existence of edge states. To elucidate the behavior of these edge states, we investigate the SU(3) system in a strip geometry. We apply periodic boundary conditions in the y-direction, and take a system of finite length in the x-direction. The system in this strip geometry is described by

$$H_{\text{strip}} = -t\sum_i [\Psi_i^{\dagger}(k_y)2\cos(k_y - \hat{A}_y)\Psi_i(k_y)$$
$$+ \Psi_i^{\dagger}(k_y)e^{-i\hat{A}_x}\Psi_{i+1}(k_y) + \Psi_{i+1}^{\dagger}(k_y)e^{i\hat{A}_x}\Psi_i(k_y)], \quad (15)$$
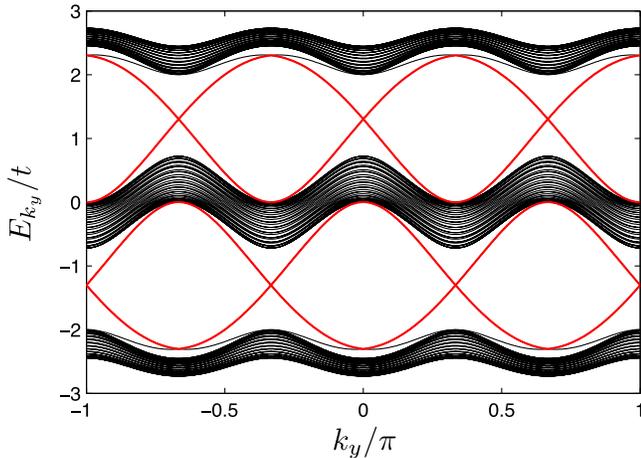
FIG. 1 (color online). The spectrum of the SU(3) model in a strip geometry. The bulk states correspond to black lines while the edge states correspond to the thick red lines. The presence of such topological edge states is implied, through the bulk-boundary correspondence, by nonzero Chern numbers.

where i now is a one-dimensional finite sum. The eigenstates of H_{strip} are plotted in Fig. 1. The spectrum exhibits characteristic topological edge states that connect the bands with different Chern numbers.

In conclusion we make a few general remarks. First, we note that while the SU(3) topological insulator constructed here relies on spin-orbit coupling of a new type and while the calculation of Chern numbers requires a new algebraic construction, its overall topological characterization resides within the existing general classification scheme [31,32] and corresponds there to a lattice quantum Hall state labeled by an integer topological index. However in contrast to solid-state systems where the absence or presence of time-reversal symmetry is an obvious physical constraint, for synthetic spin-orbit systems the notion of time-reversal symmetry does not have such a direct meaning, because the synthetic spins do not behave like real spins under time reversal. Classification of cold-atom Hamiltonians with respect to transformations of the time-reversal type can still be formulated but in a more formal way by examining the existence of an antiunitary symmetry of the Hamiltonian which may or may not have a direct physical interpretation. From this perspective, our Hamiltonian does not have such a symmetry. One can argue that in general such Chern topological insulators are much easier to realize with cold atoms than Z_2 topological insulators, because imposing an additional unphysical symmetry would require fine tuning the synthetic Hamiltonian, in contrast to the situation in the solid state where in the absence of external magnetic fields and magnetic impurities time-reversal invariance is automatically preserved. Finally, we briefly comment on the experimental realization of the SU(3) system. There exists a considerable literature on the realization of synthetic gauge fields in cold atom systems (for a review, see Ref. [16]). The gauge fields from Eq. (4) can be realized with variations of the so-called N-pod schemes [16,33]. While the N-pod schemes yield static gauge fields (as considered in this work) only, there are proposed extensions to dynamical gauge fields [34] whose study in the context of SU(3) systems have important connections with particle physics and will be an interesting avenue of future consideration.

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