Topological invariant and cotranslational symmetry in strongly interacting multi-magnon systems

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Abstract

It is still an outstanding challenge to characterize and understand the topological features of strongly interacting states such as bound states in interacting quantum systems. Here, by introducing a cotranslational symmetry in an interacting multi-particle quantum system, we systematically develop a method to define a Chern invariant, which is a generalization of the well-known Thouless–Kohmoto–Nightingle–den Nijs invariant, for identifying strongly interacting topological states. As an example, we study the topological multi-magnon states in a generalized Heisenberg XXZ model, which can be realized by the currently available experiment techniques of cold atoms (Aidelsburger et al 2013 Phys. Rev. Lett. 111, 185301; Miyake et al 2013 Phys. Rev. Lett. 111, 185302). Through calculating the two-magnon excitation spectrum and the defined Chern number, we explore the emergence of topological edge bound states and give their topological phase diagram. We also analytically derive an effective single-particle Hofstadter superlattice model for a better understanding of the topological bound states. Our results not only provide a new approach to defining a topological invariant for interacting multi-particle systems, but also give insights into the characterization and understanding of strongly interacting topological states.

1. Introduction

Topological invariants, which describe the invariant property of a topological space under homeomorphisms, are of great importance in characterizing topological matters and topological phase transitions. Weakly interacting topological states, whose universal properties do not depend on inter-particle interactions, are well understood due to the well-developed tools for treating weakly interacting systems [1–5]. However, strongly interacting topological states, whose universal properties are determined by inter-particle interactions, pose much greater challenges to both theory [6] and experiment [7]. The characterization of strongly interacting topological states is quite different from that of their weakly interacting counterparts [8, 9]. Due to the existence of strong correlations among particles, it is hard to define a topological invariant and to clarify the interplay between topological features and inter-particle interactions.

Ultracold atoms in optical lattices offer a well-controlled experimental platform to explore topological matters in a clean environment [10]. Recently, the Hofstadter–Harper model has been experimentally realized by using laser-assisted tunneling of ultracold atoms in a tilted optical potential [11, 12]. As the atom–atom interaction can be tuned by Feshbach resonances, such an atomic Hofstadter–Harper system not only opens a way to explore topological states of noninteracting atoms, but also provides new opportunity to study strongly interacting topological states.

Beyond single-particle topological states [13–19], it is of great challenge to clarify whether interacting topological states may emerge. One outstanding challenge is the absence of a well-defined topological invariant for an interacting quantum system (IQS). In this paper, we find that this problem can be solved when the system
has cotranslational symmetry: the invariance under collective translation. We demonstrate that the cotranslational symmetry naturally allows us to formulate a topological invariant, which can be used to characterize the topological features of interacting multi-particle states such as bound states (BSs). In comparison with other topological invariants, our topological invariant is intrinsic and straightforward. A well-known generalization of the Thouless–Kohmoto–Nightingale–den Nijs (TKNN) invariant [20] from noninteracting to interacting systems is by introducing the twisted boundary condition (BC) [21], which requires calculation of all many-body ground states for a continuous 2π-period of the twist angle. Another topological invariant for IQSs is given in terms of the Green’s function, which requires calculation of the Green’s function at all frequencies [22] or zero frequency [23]. Differently, our topological invariant is directly defined by using the center-of-mass (c.o.m) quasi-momentum associated with the cotranslational symmetry. We believe that our definition opens a new route to the characterization of strongly interacting topological states.

2. Topological invariant associated with cotranslational symmetry

To illustrate our idea, we first consider a generally two-dimensional (2D) quantum system with N interacting particles. The Hamiltonian reads as

$$H = \sum_{j=1}^{N} H_j + \sum_{j=1}^{N} \sum_{j'=j+1}^{N} V(|r_j - r_{j'}|).$$  

(1)

Here, \(r_j = (x_j, y_j)\) is the position of the \(j\)th particle, the single-particle Hamiltonian \(H_j\) is of translational symmetry with respect to the period \(a = (a_x, a_y)\), and the interaction \(V(|r_j - r_{j'}|)\) only depends on the inter-particle distance. Typical examples are quantum lattice models such as Hubbard lattices and quantum spin lattices. Although we concentrate on quantum lattice models, our idea can be extended to continuous models.

Given an \(N\)-particle wave function \(\psi(r_1, r_2, \ldots, r_N)\), the single-particle translation operator for the \(j\)th particle, \(T^j(\tau)\), is defined as \(T^j(\tau)\psi(r_1, r_2, \ldots, r_N) = \psi(r_1, \ldots, r_j + \tau, \ldots, r_N)\) with \(j \in \{1, 2, \ldots, N\}\). For a noninteracting system, because of the translational symmetry of each single-particle Hamiltonian \(H_j\), \(T^j(\tau)\) commutes with the whole Hamiltonian and the many-body eigenstate has a tensor product structure of \(N\) single-particle Bloch states. Therefore the independent Bloch momenta of the \(N\) particles form a set of good quantum numbers for the noninteracting Hamiltonian. However, the interaction will break the single-particle translational symmetry and make the \(N\) independent Bloch momenta no longer good quantum numbers.

We now define the cotranslation operator, \(T_\alpha(\tau)\), as

$$T_\alpha(\tau)\psi(r_1, r_2, \ldots, r_N) = \psi(r_1 + \tau a, r_2 + \tau a, \ldots, r_N + \tau a)$$

(2)

with \(\tau\) an arbitrary integer. Actually, \(T_\alpha(\tau)\) is a combination of all single-particle translation operators, \(T_\alpha(\tau) = [T^{(1)}(\tau)T^{(2)} \ldots T^{(N)}]^{\tau}\), and thus it commutes with each \(H_j\). Since \(T_\alpha(\tau)T_\alpha(\tau') = T_\alpha(\tau + \tau')\) and \([T_\alpha(\tau)]^{-1} = T_\alpha(-\tau)\), the set \(\{T_\alpha(\tau), \tau \in \mathbb{Z}\}\) forms an Abelian group (where \(\mathbb{Z}\) is the set of all integers). We call this group the cotranslation group. As all cotranslation operators commute with the interaction term, the whole Hamiltonian is invariant under the cotranslation transform,

$$[T_\alpha(\tau)]^{-1}HT_\alpha(\tau) = H,$$

(3)

which represents cotranslational symmetry.

Under cotranslational symmetry, the Hamiltonian \(H\) and \(T_\alpha(\tau)\) share a set of common eigenstates. The common eigenstates obey

$$T_\alpha(\tau)\psi(r_1, r_2, \ldots, r_N) = c_\alpha(\tau)\psi(r_1, r_2, \ldots, r_N),$$

(4)

with \(c_\alpha(\tau)\) being an eigenvalue of \(T_\alpha(\tau)\). It is easy to find \(c_\alpha(\tau)c_\alpha(\tau') = c_\alpha(\tau + \tau')\) and \([c_\alpha(\tau)]^{-1} = c_\alpha(-\tau)\).

Thus the eigenvalues could be chosen as the exponential form \(c_\alpha(\tau) = e^{i\kappa \cdot a}\) with the vector \(\kappa = (k_x, k_y)\) [24], which is a pair of good quantum numbers. Thus we have,

$$\psi(r_1 + \tau a, \ldots, r_N + \tau a) = e^{i\kappa \cdot a}\psi(r_1, \ldots, r_N),$$

(5)

which resembles the Bloch theorem for single-particle systems with translational symmetry. Therefore, the vector \(\kappa\) acts as the corresponding c.o.m quasi-momentum. Similar to the Bloch functions for single-particle systems with translational symmetry, one can define \(\psi(r_1, r_2, \ldots, r_N) = e^{i\kappa \cdot (r_1 + r_2 + \cdots + r_N)}\phi(r_1, r_2, \ldots, r_N)\) and then obtain \(\phi(r_1 + \tau a, r_2 + \tau a, \ldots, r_N + \tau a) = \phi(r_1, r_2, \ldots, r_N)\) from equation (5). We thus identify these eigenstates \(\psi(r_1, r_2, \ldots, r_N)\) as the many-body Bloch states for IQSs with cotranslational symmetry.

By exploiting the cotranslational symmetry and the many-body Bloch states, we define a topological invariant (the first Chern number). It is an integral of the Berry curvature \(F_\alpha(k_x, k_y)\) over the first Brillouin zone (BZ),
$$C_n = \frac{1}{2\pi} \int_{BZ} d\mathbf{k} \, \mathcal{F}_n(k_x, k_y),$$

(6)

where, \( \mathcal{F}_n(k_x, k_y) = \text{Im}(\langle \partial_x \phi_n | \partial_y \phi_n \rangle - \langle \partial_y \phi_n | \partial_x \phi_n \rangle) \) is determined by the Bloch state \( |\phi_n \rangle = |\phi_n(k_x, k_y)\rangle \), \( k_x \in (-\pi/a_x, \pi/a_x) \) and \( k_y \in (-\pi/a_y, \pi/a_y) \) and \( n \) is the band index. In fact, the above Chern number is a TKNN-type topological invariant. We should remark that our topological invariant is always well-defined for the band which is well-separated from other bands, that is, it is protected by the corresponding energy gaps.

3. Topological bound states in generalized Heisenberg XXZ model

3.1. A generalized Heisenberg XXZ model

We now consider a generalized 2D Heisenberg XXZ model described by the following Hamiltonian,

$$\hat{H}_1 = -J_x \sum_{l,m} \left[ (e^{i\pi N} \hat{S}_{l+1,m}^+ \hat{S}_{l,m}^- + \lambda \hat{S}_{l,m+1}^+ \hat{S}_{l,m}^-) + \text{h.c.} \right]$$

$$= V_x \sum_{l,m} \left[ \hat{S}_{l,m}^x \hat{S}_{l+1,m}^x + \lambda \hat{S}_{l,m}^x \hat{S}_{l,m+1}^x \right]$$

(7)

with the spin-1/2 operators \( \hat{S}_{l,m}^x \) and \( \hat{S}_{l,m}^y \) for the lattice site \((l, m)\). Here, \( J_x \) and \( V_x \) are the transverse and longitudinal spin-exchange couplings, respectively. And \( \lambda \) represents the ratio of the interactions between y- and x-directions. Different from the usual 2D Heisenberg XXZ model, our \( \hat{H}_1 \) includes a spatially varying phase \( 2\pi \phi \) along the x-direction.

According to the Matsubara–Matsuda mapping [25], the model \( \hat{H}_1 \) is equivalent to a hard-core Bose–Hubbard model. By introducing \(|\uparrow\rangle \leftrightarrow |0, 1\rangle \leftrightarrow |1\rangle\), \( \hat{S}_{l,m}^x \leftrightarrow \hat{b}_{l,m}^+ \leftrightarrow \hat{b}_{l,m} \) and \( \hat{S}_{l,m}^y \leftrightarrow \hat{b}_{l,m}^+ \hat{b}_{l,m} - \frac{1}{2} \) we have,

$$\hat{H} = -J_x \sum_{l,m} \left( e^{i(2\pi/3)} \hat{b}_{l,m}^+ \hat{b}_{l,m} + \lambda \hat{b}_{l,m}^+ \hat{b}_{l,m+1} + \text{h.c.} \right)$$

$$= V_x \sum_{l,m} \left[ \hat{n}_{l,m} \hat{n}_{l+1,m} + \lambda \hat{n}_{l,m} \hat{n}_{l,m+1} \right]$$

(8)

with the hard-core bosonic creation (annihilation) operators \( \hat{b}_{l,m}^+ \) and the number operator \( \hat{n}_{l,m} = \hat{b}_{l,m}^+ \hat{b}_{l,m} \). Here, \( \beta = \Phi/\pi \) and we have removed a constant energy shift. Below, we concentrate on discussing the rational flux \( \beta = p/q \) (where \( p \) and \( q \) are coprime integers) and consider a lattice of \( L_x \times L_y \) sites and \( L_y = q s \) with an odd integer \( s \).

Our model (8) can be regarded as a specific representation of the general model (1) given in section 2. The tunneling terms (the first part) in our model (8) represents the single-particle Hamiltonians \( \sum_{l} \hat{H}_1 \) in the models (1) and the second term represents the inter-particle interactions. For a rational \( \beta = p/q \), the spatially varying phase \( 2\pi \phi = 2\pi/3m \) ensures translational symmetry in the single-particle Hamiltonian. Furthermore, the periods of each single-particle Hamiltonian are \( \mathbf{a} = (\mathbf{a}_x, \mathbf{a}_y) = (1, q) \) in the unit of the lattice constants \( (d_x, d_y) \) along x- and y-directions. For noninteracting systems, the spatially varying phase associates with magnetic effects, which induces a magnetic BZ. However, the interaction term will break the single-particle translational symmetry. Therefore, our work actually generalizes the magnetic BZ from noninteracting systems to interacting ones.

3.2. Topological two-magnon excitations

The two-particle Hilbert subspace is spanned by the basis, \( B_{2D}^T = \{|l_1, m_1; l_2, m_2\} = \hat{b}_{l,m}^+ |0\rangle \), with \( 1 \leq l_1 < l_2 \leq L_x \) or \( 1 \leq l_1 = l_2 \leq L_x \) and \( 1 \leq m_1 < m_2 \leq L_y \). We then impose periodic boundary conditions (PBCs) in both x- and y-directions. By introducing \( \psi_{l_1,m_1,l_2,m_2} = \langle l_1, m_1, l_2, m_2 | \hat{b}_{l,m}^+ \hat{b}_{l,m} | \psi \rangle \), the eigenstates can be expanded as \( |\psi \rangle = \sum_{l_1,m_1,l_2,m_2} \psi_{l_1,m_1,l_2,m_2} |l_1, m_1, l_2, m_2\rangle \). The eigenvalue \( \hat{H}|\psi \rangle = E|\psi \rangle \) gives

$$E\psi_{l_1,m_1,l_2,m_2} = -V_x (e^{i2\pi/3} \psi_{l_1-1,m_1,l_2} + e^{-i2\pi/3} \psi_{l_1+1,m_1,l_2})$$

$$- J_x (e^{i2\pi/3} \psi_{l_1,m_1-1,l_2} + e^{-i2\pi/3} \psi_{l_1,m_1+1,l_2})$$

$$+ e^{i2\pi/3} \psi_{l_1,m_1,l_2-1} + e^{-i2\pi/3} \psi_{l_1,m_1,l_2+1}$$

$$+ \lambda \psi_{l_1,m_1-1} + \lambda \psi_{l_1,m_1+1}$$

$$+ \lambda \psi_{l_1,m_1,l_2-1} + \lambda \psi_{l_1,m_1,l_2+1}$$

(9)

where the PBCs require that \( \psi_{l+1,m_1,l_2,m_2} = \psi_{l,m_1+1,l_2,m_2} = \psi_{l,m_1,l_2+1,m_2} = \psi_{l,m_1,l_2,m_2+1} \), and the hard-core bosonic commutation relations require that \( \psi_{l_1,m_1,l_2,m_2} = \psi_{l_1,m_1,l_2,m_2+1} \) and \( \psi_{l_1,m_1,l_2,m_2} = 0 \).

To describe the cotranslational symmetry along the x-direction, we introduce the two-particle cotranslational operator \( \hat{T}_x^l \) as
\[ T_i^f \psi_{m_i,m_{i+1}} = \psi_{m_i+1,m_{i+2}} \]  
(10)

It is easy to find that \( HT_i^f \psi_{m_i,m_{i+1}} = T_i^f H \psi_{m_i,m_{i+1}} \) holds for arbitrary \( \psi_{m_i,m_{i+1}} \). Therefore, the Hamiltonian \( H \) commutes with \( T_i^f \) and they share a set of common eigenstates: \( \psi_{m_i,m_{i+1}} = e^{i\phi} \phi_{m_i,m_{i+1}} \), in which \( \phi_{m_i,m_{i+1}} \) is invariant under \( T_i^f \). The eigeneguation \( H \phi = E \phi \) gives

\[
E_k \phi_{m_i,m_{i+1}} = -V(x) \phi_{m_i,m_{i+1}} + \frac{\hbar^2}{2m} \frac{\partial^2 \phi_{m_i,m_{i+1}}}{\partial x^2} + \frac{\hbar^2 k^2}{2m} \phi_{m_i,m_{i+1}}.
\]

Therefore, the Hamiltonian \( H_k \) is invariant under \( T_i^f \). The eigeneguation \( H_k \phi = E_k \phi \) gives

\[
E_k \phi_{m_i,m_{i+1}} = -V(x) \phi_{m_i,m_{i+1}} + \frac{\hbar^2}{2m} \frac{\partial^2 \phi_{m_i,m_{i+1}}}{\partial x^2} + \frac{\hbar^2 k^2}{2m} \phi_{m_i,m_{i+1}}.
\]

(11)

Here, \( H_k \) denotes the \( k_x \)-block of the two-particle Hamiltonian and \( k_x = \frac{2\pi}{L_x} \alpha_x \) is the c.o.m quasi-momentum along the \( x \)-direction (with the integer \( \alpha_x \in \left[ -\frac{L_x-1}{2}, \frac{L_x-1}{2} \right] \)). Correspondingly, the PBCs require

\[
\phi_{m_i,m_{i+1}} = \phi_{m_i,m_{i+1}+L_x,m_{i+1}} = (-1)^{m_i} \phi_{m_i,m_{i+1}},\quad \text{and } \phi_{m_i,m_{i+1}+L_y,m_{i+1}} = \phi_{m_i,m_{i+1}+L_y} = \phi_{m_i,m_{i+1}+L_y} = \phi_{m_i,m_{i+1}+L_y}.\]

The c.o.m quasi-momenta are good quantum numbers and the energy spectrum. Actually, under PBCs, the c.o.m quasi-momenta are good quantum numbers and the energy spectrum. It is easy to find that \( H_k \phi = E_k \phi \), where \( H_k \phi = E_k \phi \) holds for arbitrary \( \phi_{m_i,m_{i+1}} \). Therefore, \( H_k \) and \( T_i^f \) have a common set of eigenstates, which can be written as \( \phi_{m_i,m_{i+1}} = e^{i\phi} \phi_{m_i,m_{i+1}} \), where \( \phi_{m_i,m_{i+1}} \) is invariant under \( T_i^f \). The eigeneguation \( H_k \phi = E_k \phi \) reads

\[
E_k \phi_{m_i,m_{i+1}} = -V(x) \phi_{m_i,m_{i+1}} + \frac{\hbar^2}{2m} \frac{\partial^2 \phi_{m_i,m_{i+1}}}{\partial x^2} + \frac{\hbar^2 k^2}{2m} \phi_{m_i,m_{i+1}}.
\]

(12)

In the \( k_y \)-subspace, it turns out to be \( T_i^f \phi_{m_i,m_{i+1}} = \phi_{m_i+q,m_{i+1}+q} \). It is easy to find that \( H_i \phi_{m_i,m_{i+1}} = T_i^f H_k \phi_{m_i,m_{i+1}} \), where \( H_i \phi_{m_i,m_{i+1}} \) holds for arbitrary \( \phi_{m_i,m_{i+1}} \). Therefore, \( H_i \) and \( T_i^f \) have a common set of eigenstates, which can be written as \( \phi_{m_i,m_{i+1}} = e^{i\phi} \phi_{m_i,m_{i+1}} \), where \( \phi_{m_i,m_{i+1}} \) is invariant under \( T_i^f \). The eigeneguation \( H_i \phi = E_i \phi \) reads

\[
E_i \phi_{m_i,m_{i+1}} = -V(y) \phi_{m_i,m_{i+1}} + \frac{\hbar^2}{2m} \frac{\partial^2 \phi_{m_i,m_{i+1}}}{\partial y^2} + \frac{\hbar^2 k^2}{2m} \phi_{m_i,m_{i+1}}.
\]

(13)

Here, \( k_y = \frac{2\pi}{L_y} \alpha_y \) is the c.o.m quasi-momentum along the \( y \)-direction (with the integer \( \alpha_y \in \left[ -\frac{L_y-1}{2}, \frac{L_y-1}{2} \right] \)).

In the above, we have used the conditions \( \alpha_x \in \left[ -\frac{L_x-1}{2}, \frac{L_x-1}{2} \right] \) and \( \alpha_y \in \left[ -\frac{L_y-1}{2}, \frac{L_y-1}{2} \right] \) for calculating the energy spectrum. Actually, under PBCs, the c.o.m quasi-momenta are good quantum numbers and the energy spectrum versus the c.o.m quasi-momenta can be calculated for arbitrary \( L_x \) and \( L_y \). However, due to the indistinguishability of the two magnons, the c.o.m quasi-momentum may associate with a different number of eigenstates when the total magnon number \( N \) is even and the total number of lattice sites \( L_x \) and \( L_y \) are not coprime with each other (i.e. the greatest common divisor \( \text{gcd}(N, L_x, L_y) \neq 1 \)). To make each c.o.m quasi-momentum associating with the same number of eigenstates, we set both \( L_x \) and \( L_y \) as odd integers which ensure \( \text{gcd}(N, L_x, L_y) = 1 \). On the other hand, for systems of distinguishable particles, every c.o.m quasi-momenta associates with the same number of eigenstates for arbitrary values of \( (N, L_x, L_y) \).

We now discuss the two-magnon spectrum. In figure 1, we show the whole two-magnon spectra for different \( V_x/L_x \). For sufficiently strong interactions (see figures 1(b) and (c)), there are two different kinds of bands, in which the upper bands (continuum band) correspond to scattering states and the lower bands (BS band) to bound states. While for weak interactions (see figure 1(a)), these two kinds of bands may overlap. Below, we focus on discussing strongly interacting systems, which have a significant gap between the scattering-state band and the BS band.

In figure 2(a), we show the BS spectrum for the strongly interacting system under periodic BCs. Our calculation shows that there are six subbands for \( \beta = 1/3 \). Due to there being only nearest-neighbor interactions, the BSs can be approximated by a superposition of states \( |n; m, l+1, m \rangle \) and \( |l; m, l+1, m \rangle \). As the total number of states in forms of \( |n; m, l+1, m \rangle \) and \( |l; m, l+1, m \rangle \) is \( 2L_x L_y \), there are \( N_{BS} = 2L_x L_y \) BSs in our system. Meanwhile, for a given \( \beta = p/q \), the numbers of c.o.m quasi-momenta along the \( x \)- and \( y \)-directions are \( L_x \) and \( L_y \), respectively. This indicates that the number of eigenstates in each BS subband is \( D_{BS} = L_x L_y \). Therefore, the BS spectrum includes \( N_{BS}/D_{BS} = 2q \) subbands.

Based on our calculation, the Chern numbers of the six subbands (for \( \beta = 1/3 \)) are \( (C_0, C_2, \ldots, C_6) = (-1, 2, -1, -1, 2, -1) \). The Chern numbers indicate the bulk system has a nontrivial topology. According to the bulk-edge correspondence, topological edge states will appear in the system under open BCs. So we calculate
Figure 1. Entire two-magnon spectra. Band-gap structures for (a) $V_e/J_x = 1$, (b) $V_e/J_x = 5$, and (c) $V_e/J_x = 10$. In our calculation, the parameters are chosen as $\beta = 1/3$ and $\lambda = 1.2$, and the boundary conditions are set as the periodic BC along the $x$-direction with $L_x = 51$ and the periodic BC along the $y$-direction with $L_y = 33$.

Figure 2. Two-magnon BS spectra. BS bands for (a) periodic BC along the $y$-direction with $L_y = 33$ and (b) open BC along the $y$-direction with $L_y = 34$. Both (a) and (b) choose the periodic BC along the $x$-direction with $L_x = 51$. (c) The density distribution along the $y$-direction for $A$ (red circle) with $k_x = 0$ and $B$ (blue square) with $k_x = 2\pi/3$ in (b). The other parameters are chosen as $\beta = 1/3$, $V_e/J_x = 10$ and $\lambda = 1.2$. 

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the spectrum under the open BC along the $y$-direction. In figure 2(b), in addition to the extended BSs, topological edge BSs do appear. In figure 2(c), corresponding to the two points ($A$, $B$) in figure 2(b), we show their density distributions along the $y$-direction ($\rho_y(m) = \langle \hat{n}_y(m) \rangle = \langle \sum_i \hat{n}_{i,m} \rangle$). The density distributions clearly show that these BSs do localize on the edges.

### 3.3. Topological phase transitions

The interaction ratio $\lambda$ plays an important role in the BS spectrum. If $\lambda \gg 1$ (i.e. the interaction along the $y$-direction dominates), the eigenstates of the three lowest subbands can be approximated by a superposition of $|l, m; l, m + 1\rangle$, which are called $y$-type BSs; while the eigenstates of the three higher subbands can be approximated by a superposition of $|l, m; l + 1, m\rangle$, which are called $x$-type BSs. If $\lambda \approx 1$ (i.e. $V_x \approx V_y$), the BSs are approximated by superpositions of $|l, m; l + 1, m\rangle$ and $|l, m; l, m + 1\rangle$. Otherwise, if $\lambda \ll 1$, the three lowest subbands correspond to $x$-type BSs while three higher subbands correspond to $y$-type BSs. By introducing $P_x = \sum_{l,m} |\psi_{l,m,l+1,m}|^2$ and $P_y = \sum_{l,m} |\psi_{l,m,l,m+1}|^2$, we have $P_x = 1$ ($P_y = 1$) for a perfect $x$-type ($y$-type) BS. For an arbitrary BS, we find that $P = P_x + P_y \approx 1$ (see figure 3).

In figure 4, we show the BS spectra for different $\lambda$. According to the bulk-edge correspondence, the winding number of the edge states in a specific energy gap is another topological invariant, which equals the sum of the...
Chern numbers of the bands below this gap \([26, 27]\). We find the absolute value of the winding number \(W_1\) for the edge states in the first energy gap: \(|W_1| = 1\) for \(\lambda = 0.9\) and 1.1 (see figures 4(a), (c)) and \(|W_1| = 2\) for \(\lambda = 1\) (see figure 4(b)). This means that topological phase transitions (TPT) appear in the two regions: \(0.9 < \lambda < 1\) and \(1 < \lambda < 1.1\). Our calculations show that the Chern numbers for the lowest subband are \(C_i = (-1, 2, -1)\) for \(\lambda = (0.9, 1, 1.1)\), which are consistent with the winding numbers for the corresponding edge states.

According to the topological band theory \([1, 2]\), TPT associate with gap closures. For a finite system, a gap closure corresponds to a gap minimum, which approaches zero when the system size increases. In figure 5, we show the topological phase diagram for the first BS subband.

### 3.4. Effective single-particle Hofstadter superlattices

Under strong interactions \(\|J_x / V_x\| \ll 1\), a BS can be regarded as a quasi-particle. By treating the tunneling as a perturbation to the interaction and implementing the Schrieffer–Wolff transformation \([28]\), the system obeys an effective single-particle model (see appendix C).
are standard Hofstadter Hamiltonians, and the operators $\hat{A}^\dagger_{lm}$ and $\hat{B}^\dagger_{lm}$ create a particle in states $|l, m; l + 1, m\rangle$ and $|l, m; l, m + 1\rangle$, respectively. In figure 7(a), we show the lattice structure, in which the green and red circles respectively represent the sublattices A and B. Actually, $\hat{H}_A$ and $\hat{H}_B$ are standard Hofstadter Hamiltonians, and $\hat{H}_{AB}$ describes the coupling between the two sublattices.

Now we discuss the quasi-particle spectrum. Under the periodic BC along the x-direction, through the Fourier transformation: $\hat{A}^\dagger_{lm} = \frac{1}{\sqrt{\eta_e}} \sum_k e^{i k_x x} a^\dagger_{k, l}$ and $\hat{B}^\dagger_{lm} = \frac{1}{\sqrt{\eta_e}} \sum_k e^{i k_x x} b^\dagger_{k, l}$, the system (14) becomes block diagonalized. The eigenstates $|\Psi(k_x)\rangle = [\psi^A_{k}(k_x) \hat{A}^\dagger_{k, l} + \psi^B_{k}(k_x) \hat{B}^\dagger_{k, l}]|0\rangle$ obey the coupled Harper equations,

$$E\psi_m = \begin{bmatrix} J^A & -J_m e^{i\Delta_x/2} \\ -J_m^{-1} e^{-i\Delta_x/2} & J^B \end{bmatrix} \psi_{m+1} - \begin{bmatrix} J^A & 0 \\ -J_m^{-1} e^{-i\Delta_x/2} & J^B \end{bmatrix} \psi_m,$$

(15)

with $E' = E/\eta_e$, $\psi_m = [\psi^A_m, \psi^B_m]^T$, $J^A = 2\lambda^2$, $J^B = \lambda$, $\Delta_x = \epsilon_x = \epsilon_m = \epsilon_m = \epsilon_y + (4/\lambda) \cos(4\pi \beta m - k_x) + 2\cos(4\pi \beta m - k_x)$, $\epsilon_m = \epsilon_y + (4/\lambda) \cos(4\pi \beta m + \pi \beta - k_x)$, and $J_m = 2J_{xy} \cos(2\pi \beta m + \pi \beta - k_x)/2$.

In figure 6, we show the energy spectra for the effective model and the original model under PBCs. There are only minor differences between the red solid lines for the effective model and the black dots for the original model. For large $V_\perp /J_x$, the red solid lines and the black dots almost completely overlap, that is, the two spectra are almost the same. In figures 7(b), (c), (d), we show the spectrum versus $\beta$. At $\lambda = 0.8$ and 1.2, the butterfly-like spectrum includes two separated parts. When $\lambda \to 1$, the gap between the two parts gradually vanishes. Finally, at $\lambda = 1$, the two parts merge into one butterfly. Actually, such a spectrum deformation can be induced by tuning the tunneling ratio $J / K$ of the spinor Hofstadter model (16).

3.5 Experimental possibility

In this section, we briefly discuss the experimental possibility. Using laser-assisted tunneling of two-component Bose atoms in a tilted optical lattice, one can realize a 2D interacting spinor Hofstadter model [11, 12], which is governed by the following Hamiltonian (see appendix A),

$$\hat{H}_B = -\sum_{l,m,\sigma} [K e^{i\alpha,\sigma,\Phi} \hat{a}^\dagger_{l+1, m, \sigma} \hat{a}_{l, m, \sigma} + \text{h.c.}] - \sum_{l,m,\sigma} [\hat{J} a^\dagger_{l, m+1, \sigma} \hat{a}_{l, m, \sigma} + \text{h.c.}] + \sum_{l,m,\sigma,\sigma' \neq \sigma} \frac{1}{2} U_{\sigma,\sigma'} \hat{n}_{l,m,\sigma} \hat{n}_{l,m,\sigma'} - \delta_{\sigma,\sigma'} \hat{\sigma}_{l,m},$$

(16)

with the lattice index $(l, m)$, the component index $\sigma \in \{\uparrow, \downarrow\}$, the creation (annihilation) operators $\hat{a}^\dagger_{l, m, \sigma}$ ($\hat{a}_{l, m, \sigma}$), and the number operator $\hat{n}_{l,m,\sigma} = \hat{a}^\dagger_{l,m,\sigma} \hat{a}_{l,m,\sigma}$. Here, $U_{\sigma,\sigma'}$ is the on-site interaction whose strength can be tuned via Feshbach resonances [29, 30], and $K$ and $J$ are respectively the tunneling energies along x- and y-directions. The tunneling along the x-direction involves an additional spin- and spatial-dependent phase $\phi_{l,m} = \alpha_\sigma m \Phi$ with $\alpha_1 = 1$ and $\alpha_2 = -1$.

In the strong interaction regime with unit filling, by using second-order perturbation theory [31], one can map the model (16) onto the 2D generalized Heisenberg XXZ model (7) (see appendix B) with the parameters $J_x = 2K^2/|U|$, $J_y = \lambda J_x$, $V_x = 4K(1/|U| + 1/|U| - 1/|U|)$, $V_y = \lambda V_x$, and $\lambda = V_y /V_x = J^2 /K^2$.

Selective magnon excitations can be prepared by using a line-shaped laser beam generated with a spatial light modulator [32, 33]. The two-magnon bound states can be observed by using an in situ correlation measurement [33]. Furthermore, one can explore TPT by varying $\lambda$ and $V_\perp /J_x$, which are respectively determined by the
tunneling ratio $J/K$ and the two interaction ratios $\langle U_{\uparrow \uparrow}/U_{\uparrow \downarrow} , U_{\uparrow \downarrow}/U_{\uparrow \uparrow}\rangle$ of the interacting spinor Hofstadter model \cite{16}.

It is worth mentioning that the interacting spinor Hofstadter model can be realized by two-component systems of either bosons or fermions. Our above discussions concentrate on systems realized by two-component bosons, whose inter-particle interactions are described by three different s-wave scattering lengths, which breaks time-reversal symmetry. However, for systems realized by fermions, it is possible to keep time-reversal-invariance in the Hofstadter–Hubbard model \cite{34, 35, 36}.

In the end of this section, we discuss the possibility of directly realizing the hard-core Bose–Hubbard model \cite{08}. Using laser-assisted tunneling of spinless Bose atoms in a tilted optical lattice, one can realize the tunneling terms (the first part) of equation \cite{08}. On the other hand, one may use dipole–dipole interactions to introduce nearest-neighbor interactions. If on-site interactions are sufficiently strong, the system can be described by the hard-core Bose–Hubbard model. However, in addition to nearest-neighbor interactions, it is unavoidable to include next-nearest-neighbor interactions which do not appear in our model \cite{08}.

4. Conclusion and discussion

In summary, from cotranslational symmetry (collectively translational invariance), we introduce an intrinsic topological invariant for interacting multi-particle quantum systems. Our topological invariant is defined as an integral of Berry curvature over the first Brillouin zone expanded by the c.o.m quasi-momentum. Our definition generalizes the well-known TKNN invariant \cite{20} and it always works for bands well-separated from others. As an application, we use our topological invariant to study the two-magnon excitations in a generalized 2D Heisenberg XXZ model. We explore the nontrivial topology of these excitations and demonstrate the emergence of topological edge BSs. We further give the topological phase diagram for the lowest BS subband. To understand the topological BSs, we derive an effective single-particle model described by a Hofstadter superlattice with two coupled standard Hofstadter sublattices. We also discuss the possible realization of our model via current cold-atom experimental techniques.

Our work studies the interacting two-body topological physics in a 2D quantum lattice model. During the submission/review procedure of this work (arXiv:1611.00205), several works have appeared on the interacting two-body topological physics in 1D quantum lattice models \cite{37, 38, 39, 40}. In [37], the authors explore the topological states of two interacting bosons in the Su–Schrieffer–Heeger (SSH) model. In [38], the authors predict the existence of two-photon topological edge states in the SSH model and map the 1D two-particle system onto a 2D single-particle system. In [39], the authors study the multihole topological states of interacting fermions in the SSH model. In [40], the authors explore the multi-particle Wannier states and the Thouless pumping of two interacting bosons in a Rice–Mele model. On the other hand, one may map a general 2D single-particle system...
onto a 1D two-particle system [41]. In this viewpoint, our 2D two-particle system is equivalent to a 1D four-particle system with complicated tunneling and interaction configurations.

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Appendix A. Realization of the interacting spinor Hofstadter model

In this section, we give a detailed derivation of the interacting spinor Hofstadter model. Based upon the approach for treating noninteracting spinless bosons [12], we generalize it to deal with interacting two-component bosons.

We consider an ultracold two-component Bose gas confined in a 2D optical lattice potential,

$$V_{\text{int}}(r) = \frac{V_0}{2} \cos \left( \frac{2\pi r_x}{\lambda_{\alpha}} \right) + \frac{V_0}{2} \cos \left( \frac{2\pi r_y}{d_{\alpha}} \right),$$  \hspace{1cm} (A.1)

with $r = (x, y)$ and $d_{\alpha} = \lambda_{\alpha}/2$. Here, $\lambda_{\alpha}$ and $V_0$ are respectively the wavelength and lattice depth along the $\alpha$-direction (where $\alpha = x, y$). A gradient magnetic field along the $x$-direction is used to generate a spin-dependent
linear potential,
\[ V_{\text{d}x} = \frac{\Delta}{d_x} \]

with the amplitude \( \Delta \). Given the bare coupling along the \( x \)-direction \( t_x \) when \( \Delta \gg t_x \), the tunneling along the \( x \)-direction is inhibited and can be restored by a pair of far-detuned running-wave beams,
\[ V_{K} (r, t) = \Omega \cos(k' \cdot r - \omega t), \]

with \( \omega = \omega_1 - \omega_2 = \Delta/h \) and \( k' = k_1 - k_2 = (k'_x, k'_y) \), see figure A1.

If the atom–atom interactions are dominated by two-body interactions, the many-body Hamiltonian includes two parts: a one-body part for single-particle contributions and a two-body part for atom–atom interactions. The single-particle Hamiltonian reads,
\[ \hat{H}_0 = \frac{\hat{p}^2}{2M} + V_{\text{lin}}(r) + V_{\text{d}x}(r) + V_{K}(r, t). \]

Here, \( \hat{p} = (\hat{p}_x, \hat{p}_y) \) and \( M \) is the atomic mass. Under ultralow temperature, the atom–atom interaction is described by the \( s \)-wave scattering and the many-body Hamiltonian reads,
\[ \hat{H} = \int d^2r [\hat{\psi}^\dagger (r) \hat{\psi}_0 (r)] + \sum_{\sigma_1, \sigma_2} \frac{1}{2} g_{\sigma_1 \sigma_2} \int d^2r [\hat{\psi}_{\sigma_1}^\dagger (r) \hat{\psi}_{\sigma_2}^\dagger (r) \hat{\psi}_{\sigma_2} (r) \hat{\psi}_{\sigma_1} (r)], \]

with the field operators \( \hat{\psi}^\dagger (r) = [\hat{\psi}_1^\dagger (r), \hat{\psi}_2^\dagger (r)] \), which creates a boson at position \( r \) with states \( |\uparrow\rangle \) and \( |\downarrow\rangle \). The interaction strength is given as \( g_{\sigma_1 \sigma_2} = \frac{4\pi\hbar^2}{M} a_{\alpha_1 \alpha_2} \), with \( a_{\alpha_1 \alpha_2} \) denoting the \( s \)-wave scattering length between components \( \sigma_1 \) and \( \sigma_2 \). Introducing \( \gamma_1 = 1 \) and \( \gamma_2 = -1 \), the many-body Hamiltonian becomes
\[ \hat{H} = \sum_{\sigma} \int d^2r [\hat{\psi}_{\sigma_0}^\dagger (r) \hat{\psi}_{\sigma_0} (r)] + \sum_{\sigma_1, \sigma_2} \frac{1}{2} g_{\sigma_1 \sigma_2} \int d^2r [\hat{\psi}_{\sigma_1}^\dagger (r) \hat{\psi}_{\sigma_2}^\dagger (r) \hat{\psi}_{\sigma_2} (r) \hat{\psi}_{\sigma_1} (r)], \]

with
\[ \hat{h}_{0, \sigma} = \frac{\hat{p}^2}{2M} + V_{\text{lin}}(r) + \gamma_{\sigma} \frac{\Delta}{d_x} + V_{K}(r, t). \]
Although the system may involve multiple bands, we assume our system only involves the lowest band which can be realized when the optical lattice is sufficiently deep.

Now we consider the Wannier–Stark–Wannier (WS-W) functions for the lowest band,

$$\phi_\sigma (\mathbf{r} - \mathbf{r}_{l,m}) = \phi^{\text{WS}}_\sigma (x - x_l) \phi^{\text{WS}}_\sigma (y - y_m),$$  \hspace{1cm} (A.8)

with $\mathbf{r}_{l,m} = (x_l, y_m) = (ld_x, md_y)$. Define $\hat{h}_0 = \frac{k^2}{2m} + \frac{V}{2} \cos \left( \frac{x}{d_x} \alpha \right)$ for $\alpha = x$ and $y$, we have $\phi^{\text{WS}}_\sigma (x - x_l)$ being the Wannier-Stark function for $\hat{h}_x$, $\alpha = \alpha_x \Delta x$, while $\phi^{\text{WS}}_\sigma (y - y_m)$ being the Wannier function for $\hat{h}_y$. By using the Wannier functions $\phi^{\text{WS}}_\sigma (x - x_l)$ for $\hat{h}_x$, the Wannier-Stark functions $\phi^{\text{WS}}_\sigma (x - x_l)$ can be expanded as

$$\phi^{\text{WS}}_\sigma (x - x_l) = \sum_j I_{l,j} (\gamma_\sigma) \phi^{\text{WS}}_\sigma (x - x_l),$$  \hspace{1cm} (A.9)

with $\gamma_\sigma = \alpha_x 2 t_x / \Delta$ and $I_j (z)$ being the $\nu$-order Bessel function of the first kind, where the bare tunneling strengths along x- and y-directions are denoted as $t_x$ and $t_y$, respectively.

By using the WS-W basis, the field operators can be expanded as

$$\hat{\psi}^\dagger \sigma (\mathbf{r}) = \sum_{l,m} \phi^{\text{WS}}_\sigma (\mathbf{r} - \mathbf{r}_{l,m}) \hat{a}^\dagger_{l,m,\sigma},$$  \hspace{1cm} (A.10)

where $\hat{a}^\dagger_{l,m,\sigma}$ creates a $\sigma$-component boson at the $(l, m)$th lattice site. Thus the many-body Hamiltonian reads

$$\hat{H} = \sum_{l',m',l,m} t^{\text{WS}}_{l,m;l',m'} \hat{a}^\dagger_{l',m',\sigma} \hat{a}_{l,m,\sigma} + \sum_{l',m',l,m} V^{\text{WS}}_{l,m;l',m'} (t) \hat{a}^\dagger_{l',m',\sigma} \hat{a}_{l,m,\sigma}
+ \sum_{l',m',l,m,l',m'} U^{\text{WS}}_{l,m;l',m',l',m'} \hat{a}^\dagger_{l',m',\sigma} \hat{a}^\dagger_{l,m,\sigma} \hat{a}_{l',m',\sigma} \hat{a}_{l,m,\sigma},$$  \hspace{1cm} (A.11)

with the parameters

$$t^{\text{WS}}_{l,m;l',m'} = \int d^2 \mathbf{r} \phi^{\text{WS}}_\sigma (\mathbf{r} - \mathbf{r}_{l,m}) (\hat{h}_{x} + \hat{h}_{y}) \phi^{\text{WS}}_\sigma (\mathbf{r} - \mathbf{r}_{l',m'}),$$

$$V^{\text{WS}}_{l,m;l',m'} (t) = \int d^2 \mathbf{r} \phi^{\text{WS}}_\sigma (\mathbf{r} - \mathbf{r}_{l,m}) V_{\mathbf{r}} (\mathbf{r}, t) \phi^{\text{WS}}_\sigma (\mathbf{r} - \mathbf{r}_{l',m'}),$$

$$U^{\text{WS}}_{l,m;l',m',l',m'} = \frac{1}{2} g_{l,m} \int d^2 \mathbf{r} \int d^2 \mathbf{r}' \phi^{\text{WS}}_\sigma (\mathbf{r} - \mathbf{r}_{l,m}) \phi^{\text{WS}}_\sigma (\mathbf{r} - \mathbf{r}_{l',m'}) \phi^{\text{WS}}_\sigma (\mathbf{r}' - \mathbf{r}_{l',m'}) \phi^{\text{WS}}_\sigma (\mathbf{r}' - \mathbf{r}_{l,m}).$$  \hspace{1cm} (A.12)

Under the single-band tight-binding (SBTB) approximation, we have

$$t^{\text{WS}}_{l,m;l',m'} = \alpha_x \Delta_{l,l'} \delta_{m,m'} + t^\text{SB} (\epsilon_{m' + 1} - \epsilon_{m - 1}),$$

$$U^{\text{WS}}_{l,m;l',m',l',m'} = \frac{1}{2} U \delta_{l,l'} \delta_{m,m'} \delta_{l,l'} \delta_{m,m'} \delta_{l,l'} \delta_{m,m'},$$  \hspace{1cm} (A.13)

with

$$U = \frac{g_{l,m}}{2} \int d^2 \mathbf{r} |\phi^{\text{WS}}_\sigma (\mathbf{r}) \phi^{\text{WS}}_\sigma (\mathbf{r})|^2 \int d^2 \mathbf{r}' |\phi^{\text{WS}}_\sigma (\mathbf{r}') \phi^{\text{WS}}_\sigma (\mathbf{r}')|^2.$$  \hspace{1cm} (A.15)

The matrix elements of $V_{\mathbf{r}} (\mathbf{r}, t)$ are given as

$$V^{\text{WS}}_{l,m;l',m'} (t) = \Omega \int d^2 \mathbf{r} \int d^2 \mathbf{r}' \phi^{\text{WS}}_\sigma (\mathbf{r} - \mathbf{r}_{l,m}) \phi^{\text{WS}}_\sigma (\mathbf{r}' - \mathbf{r}_{l',m'}) \phi^{\text{WS}}_\sigma (\mathbf{r}' - \mathbf{r}_{l,m}) \phi^{\text{WS}}_\sigma (\mathbf{r}' - \mathbf{r}_{l',m'}),$$

with $\theta_{l,m'} = \omega t - \phi_{l,m'}$ and $\phi_{l,m'} = l' \phi_{x} + m' \phi_{y}$ with $\phi_{x} = k_{x} d_{x}$ and $\phi_{y} = k_{y} d_{y}$. Define

$$t^{\text{WS}}_{\sigma, l,m', l,m'} = \int d^2 \mathbf{r} \phi^{\text{WS}}_\sigma (\mathbf{r}) \phi^{\text{WS}}_\sigma (\mathbf{r} - \mathbf{r}_{l,m'}),$$

$$t^{\Sigma, l,m', l,m'} = \int d^2 \mathbf{r} \phi^{\text{WS}}_\sigma (\mathbf{r}) \phi^{\text{WS}}_\sigma (\mathbf{r} - \mathbf{r}_{l,m'}),$$

as $\cos(k_{x} x + k_{y} y - \theta_{l,m'}) = \cos(k_{x} x) \cos(k_{y} y) \cos(\theta_{l,m'}) + \cos(k_{x} x) \sin(k_{y} y) \sin(\theta_{l,m'}) + \sin(k_{x} x) \cos(k_{y} y) \cos(\theta_{l,m'}) - \sin(k_{x} x) \sin(k_{y} y) \cos(\theta_{l,m'})$, we have

$$\cos(k_{x} x + k_{y} y - \theta_{l,m'}) = \cos(k_{x} x) \cos(k_{y} y) \cos(\theta_{l,m'}) + \cos(k_{x} x) \sin(k_{y} y) \sin(\theta_{l,m'}) + \sin(k_{x} x) \cos(k_{y} y) \cos(\theta_{l,m'}) - \sin(k_{x} x) \sin(k_{y} y) \cos(\theta_{l,m'}).$$
where
\[
I_{m-m}^{\cos} = \delta_{m}^{m} f_{m}^{m} + \delta_{m-1} f_{m-1}^{m} + \delta_{m+1} f_{m+1}^{m},
\]
\[
I_{m-m}^{\sin} = \delta_{m}^{m} g_{m}^{m} + \delta_{m-1} g_{m-1}^{m} + \delta_{m+1} g_{m+1}^{m},
\]
\[
I_{m-m}^{\cos} = \delta_{m}^{m} f_{m}^{m} + \delta_{m-1} f_{m-1}^{m} + \delta_{m+1} f_{m+1}^{m},
\]
\[
I_{m-m}^{\sin} = \delta_{m}^{m} g_{m}^{m} + \delta_{m-1} g_{m-1}^{m} + \delta_{m+1} g_{m+1}^{m},
\]
(A.18)

There are several different types of Wannier functions, it is better to use the maximally localized Wannier functions for constructing $\phi^{\text{mf}}(x-x_j)$ and $\phi^{\text{mf}}(y-y_j)$. The symmetry of the lattice potential implies the symmetric nature of the maximally localized Wannier functions [42] (i.e. they are either symmetric or antisymmetric). Therefore, under the SBTB approximation, we have the following identities: $I_{0,0}^{x,y} = 0$, $I_{0,0}^{x,s} = 0$, and $I_{1,0}^{x,x} \cos(\theta_{1,m}) + I_{1,0}^{x,x} \sin(\theta_{1,m}) = I_{1,0}^{x,x} \cos(\theta_{1,m}) + I_{1,0}^{x,x} \sin(\theta_{1,m})$. As $I_{0,0}^{x,y}$ is $\sigma$-independent, one can define $I_{0}^{x} = I_{0,0}^{x} + I_{0,0}^{y}$, therefore one can obtain
\[
V_{m,m',l,m}^{\cos} = \Omega_{m}^{\cos} \delta_{m}^{m} (\delta_{0} I_{0}^{x} \cos(\theta_{1,m}))
\]
\[
+ \delta_{m}^{m} I_{1,0}^{x,x} \cos(\theta_{1,m}) + I_{1,0}^{x,x} \sin(\theta_{1,m})
\]
\[
+ \delta_{m-1} f_{m-1}^{m} + \delta_{m+1} f_{m+1}^{m},
\]
(A.19)

From equations (A.11), (A.13), (A.14), and (A.19), the SBTB Hamiltonian can be written as
\[
\hat{H} = \hat{H}^{D} + \hat{H}^{ODx} + \hat{H}^{ODy} + \hat{H}^{DI},
\]
(A.20)

with
\[
\hat{H}^{D} = \sum_{l,m,\sigma} \left[ \alpha_{l} \Delta_{l} + \Omega_{m}^{\cos} \delta_{m}^{m} \cos(\theta_{1,m}) \hat{n}_{m,\sigma} \right],
\]
(A.21)
\[
\hat{H}^{ODx} = \sum_{l,m,\sigma} \Omega_{m}^{\cos} \delta_{m}^{m} (\delta_{0} I_{0}^{x} \cos(\theta_{1,m})) + \text{h.c.},
\]
(A.22)
\[
\hat{H}^{ODy} = \sum_{l,m,\sigma} \Omega_{m}^{\cos} \delta_{m}^{m} (\delta_{0} I_{0}^{y} \sin(\theta_{1,m})) + \text{h.c.},
\]
(A.23)
\[
\hat{H}^{DI} = \sum_{l,m,n,\sigma} \frac{1}{2} \Omega_{m}^{\cos} \delta_{m}^{m} \hat{n}_{m,\sigma}(\hat{n}_{m,\sigma} - \delta_{m,\sigma}),
\]
(A.24)

where $\hat{n}_{m,\sigma} = \hat{a}_{m,\sigma}^{\dagger} \hat{a}_{m,\sigma}$ and $\hat{t}_{1,m,\sigma}^{x} = \hat{a}_{m,\sigma}^{\dagger} \cos(\theta_{1,m}) + \hat{a}_{m,\sigma}^{-}\sin(\theta_{1,m})$.

The time dependence of the diagonal term $\hat{H}^{D}$ can be eliminated via a unitary transformation,
\[
\hat{U} = \exp \left( \sum_{l,m,\sigma} \lambda_{l,m,\sigma} \hat{n}_{m,\sigma} \right),
\]
(A.25)

where
\[
\lambda_{l,m,\sigma} = -\alpha_{l} \omega t - \frac{\Omega_{m}^{\cos}}{\omega_{l}} \hat{t}_{1,m}^{x} \sin(\theta_{1,m}) + \theta_{l},
\]
(A.26)

is real and time-dependent. For convenience, we introduce a spin-dependent phase $\theta_{l}$ whose value will be determined below. The Hamiltonian in the rotating frame is given as $\hat{H}' = \hat{U} \hat{H} \hat{U}^{-1} - i \hbar \hat{U}'(\partial_{t} \hat{U})$. For resonant driving (i.e. $\hbar \omega = \Delta$), we have $\hat{U}' \hat{H} \hat{U} - i \hbar \partial_{t} \hat{U} = 0$. Thus, $\hat{H}'$ becomes
\[
\hat{H}' = \hat{H}^{D} + \hat{H}^{ODx} + \hat{H}^{ODy} + \hat{H}^{DI}.
\]
(A.27)

Using the bosonic identity $e^{-i \alpha \hat{a}_{m}^{\dagger} \hat{a}_{m}^{\dagger}} e^{i \alpha \hat{a}_{m}^{\dagger} \hat{a}_{m}^{\dagger}}$, we have $\hat{U}' \hat{a}_{m,\sigma}^{\dagger} \hat{U} = e^{-i \lambda_{m,\sigma} \hat{a}_{m,\sigma}}$ and $\hat{U}' \hat{a}_{m,\sigma}^{\dagger} \hat{U} = e^{-i \lambda_{m,\sigma} \hat{a}_{m,\sigma}}$. Consequently, one can find
\[
\hat{U}' \hat{a}_{m+1,\sigma}^{\dagger} \hat{U} = e^{i \lambda_{m+1,\sigma} \hat{a}_{m+1,\sigma}^{\dagger} \hat{a}_{m,\sigma}},
\]
(A.28)
\[
\hat{U}' \hat{a}_{m,\sigma}^{\dagger} \hat{U} = e^{i \lambda_{m,\sigma} \hat{a}_{m,\sigma}^{\dagger} \hat{a}_{m,\sigma}},
\]
(A.29)

with the time-dependent phases
\[
\lambda_{l,m,\sigma} - \lambda_{l+1,m,\sigma} = \alpha_{l} \omega t - \theta_{l} - \Gamma_{x} \cos \left( \omega t - \phi_{l-m} - \frac{\phi_{l}}{2} \right),
\]
(A.30)
\[
\lambda_{l,m,\sigma} - \lambda_{l,m+1,\sigma} = -\Gamma_{x} \cos \left( \omega t - \phi_{l-m} - \frac{\phi_{l}}{2} \right),
\]
(A.31)

Here, $\Gamma_{x} = \frac{\Omega_{m}^{\cos}}{\omega_{l}} \hat{t}_{1,m}^{x} \sin \left( \frac{\phi_{l}}{2} \right)$ with $\alpha = x$ and $y$. Using the variant of the Jacobi–Anger identity, $e^{-iz \cos(\theta)} = e^{-iz \sin(\theta-z)} = \sum_{j} J_{j}(z) e^{i\theta} \left( \cos(\theta) - z \right)$, the phase factors are given as
\[
e^{i(\lambda_{\alpha_{\beta_0}} - \lambda_{\alpha_{\beta}} - \lambda_{\alpha_{\beta} + 1})\omega t} = \sum_l U_l(\Gamma_{\alpha}) e^{i(\sigma_{\alpha_0} - \sigma_{\beta_0} - \sigma_{\beta} - \sigma_{\beta + 1})\omega t} e^{-i\phi_{\beta_0}/2} e^{-i\phi_{\beta}/2},
\]
(A.32)

\[
e^{i(\lambda_{\alpha_{\beta_0}} - \lambda_{\alpha_{\beta}} - \lambda_{\alpha_{\beta} + 1})\omega t} = \sum_l j_l(\Gamma_{\alpha}) e^{i\omega t - i\phi_{\beta_0}/2} e^{-i\phi_{\beta}/2}.
\]
(A.33)

Therefore the off-diagonal terms of the Hamiltonian $\hat{H}^!$ become

\[
\hat{U}^{\dagger} \hat{H}^{\text{OD}} \hat{U} = \sum_{lm,\sigma} [K^l_{lm}(t) \hat{a}^{\dagger}_{lm+1,\sigma} \hat{a}_{lm,\sigma} + \text{h.c.}]
\]
(A.34)

\[
\hat{U}^{\dagger} \hat{H}^{\text{OD}} \hat{U} = \sum_{lm,\sigma} [U_{lm}(t) \hat{a}^{\dagger}_{lm+1,\sigma} \hat{a}_{lm,\sigma} + \text{h.c.}]
\]

with

\[
K^l_{lm}(t) = \Omega^l_0 I^l_{lm,\sigma} e^{i\omega t} e^{-i\phi_{\beta_0}/2} e^{-i\phi_{\beta}/2}.
\]
(A.36)

\[
j_{lm}(t) = t' \sum_l j_l(\Gamma_{\alpha}) e^{i\omega t - i\phi_{\beta_0}/2} e^{-i\phi_{\beta}/2}.
\]
(A.37)

Time-averaging over a period of $2\pi/\omega$ and using the identity $\frac{1}{2\pi/\omega} \int_0^{2\pi/\omega} dt \ e^{i\omega t} = \delta_{r,0}$ (for any integer $r$), one can obtain

\[
\begin{cases}
\frac{1}{2\pi/\omega} \int_0^{2\pi/\omega} dt \ K^l_{lm}(t) = e^{i\omega \phi_{\beta_0} \phi_{\beta}} \tilde{K}^l_{lm}, \\
\frac{1}{2\pi/\omega} \int_0^{2\pi/\omega} dt \ j_{lm}(t) = J.
\end{cases}
\]

Here, $J = t' j_0(\Gamma_{\alpha})$ and the $\sigma$-dependent constant $\tilde{K}^l_{lm}$ is given as

\[
\tilde{K}^l_{lm} = \frac{1}{2} \Omega^l_0 \ e^{-i\phi_{\beta_0}/2} [I^l_{\alpha_{\beta},\sigma} \ e^{i\phi_{\beta_0}/2} + I^l_{\alpha,\sigma} \ e^{-i\phi_{\beta_0}/2}]
\]
with the notation $I^l_{\alpha,\sigma} = I_{\alpha,\sigma}^{\text{cos}} + i I_{\alpha,\sigma}^{\text{sin}}$. Notice that $(I^l_{\alpha,\sigma})^* = e^{-i\phi_{\beta}} I^l_{\alpha,\sigma}$, if we define

\[
\frac{1}{2} \Omega^l_0 [I^l_{\alpha,\sigma} j_0(\Gamma_{\alpha}) - I^l_{\alpha,\sigma} j_0(\Gamma_{\alpha})] = K e^{i\theta_k}
\]
with $K > 0$ and $\theta_k \in (-\pi, \pi]$, we have

\[
\begin{cases}
\tilde{K}^l_{lm} = K e^{i(\phi_{\beta} - \phi_{\beta_0})} \\
\tilde{K}^l_{lm} = K e^{-i(\phi_{\beta} - \phi_{\beta_0})}
\end{cases}
\]
(A.41)

The undetermined phases $\theta_0$ are thus given as $\theta_1 = \theta_k$ and $\theta_1 = -\theta_k$ such that $\tilde{K}^l_{lm} = \tilde{K}^l_{lm} < 0$. Thus the effective Hamiltonian in the rotating frame $\hat{H}_{\text{eff}} = \frac{1}{2\pi/\omega} \int_0^{2\pi/\omega} dt \ \hat{H}^!$ is given as

\[
\hat{H}_{\text{eff}} = \sum_{lm,\sigma} [K e^{i\omega \phi_{\beta_0} \phi_{\beta}} \hat{a}^{\dagger}_{lm+1,\sigma} \hat{a}_{lm,\sigma} + \text{h.c.}] + \sum_{lm,\sigma} [j_{lm} \hat{a}^{\dagger}_{lm+1,\sigma} \hat{a}_{lm,\sigma} + \text{h.c.}]
\]

\[
+ \sum_{lm,\sigma} \frac{1}{2} U_{\alpha_{\beta_0}} \hat{a}_{lm,\sigma} \hat{a}_{lm,\sigma} (\hat{a}_{lm,\sigma} - \delta_{\alpha_{\beta_0}}).
\]
(A.42)

Through a time-independent unitary transformation,

\[
\hat{U}' = \exp\left(i \sum_{lm,\sigma} \lambda'_{lm,\sigma} \hat{a}_{lm,\sigma} \right),
\]
(A.43)

where $\lambda'_{lm,\sigma} = \alpha_{\beta} \frac{1}{2} \phi_1 l_1 - \beta_0 \frac{1}{2} \phi_1 l_1 L_{\sigma} - m \pi$, one can change the sign of $K$ and $J$. Since $\hat{U}^{\dagger} \hat{a}^{\dagger}_{lm,\sigma} \hat{U}' = e^{-i\lambda'_{lm,\sigma}} \hat{a}^{\dagger}_{lm,\sigma}$ and $\hat{U}^{\dagger} \hat{a}_{lm,\sigma} \hat{U}' = e^{i\lambda'_{lm,\sigma}} \hat{a}_{lm,\sigma}$, we have

\[
\hat{U}^{\dagger} \hat{a}^{\dagger}_{lm+1,\sigma} \hat{a}_{lm,\sigma} \hat{U}' = e^{i\lambda_{lm,\sigma}^\prime - \lambda_{lm+1,\sigma}^\prime} \hat{a}^{\dagger}_{lm+1,\sigma} \hat{a}_{lm,\sigma},
\]
(A.44)

\[
\hat{U}^{\dagger} \hat{a}_{lm+1,\sigma} \hat{a}_{lm,\sigma} \hat{U}' = e^{i\lambda_{lm,\sigma}^\prime - \lambda_{lm+1,\sigma}^\prime} \hat{a}_{lm+1,\sigma} \hat{a}_{lm,\sigma},
\]
(A.45)

with the phases

\[
\lambda_{lm,\sigma}^\prime - \lambda_{lm+1,\sigma}^\prime = \alpha_0 (\pi - l_1 \phi_1),
\]
(A.46)

\[
\lambda_{lm,\sigma}^\prime - \lambda_{lm+1,\sigma}^\prime = \pi.
\]
(A.47)
Thus the effective Hamiltonian becomes
\[ \hat{H}_\text{eff} = - \sum_{l,m,\sigma} \left[ K e^{i\alpha,m\eta^0} \hat{a}_{l+1,m,\sigma}^\dagger \hat{a}_{l,m,\sigma} + \text{h.c.} \right] - \sum_{l,m,\sigma} \left[ J \hat{a}_{l,m+1,\sigma}^\dagger \hat{a}_{l,m,\sigma} + \text{h.c.} \right] + \frac{1}{2} \sum_{l,m,n,\sigma_1,\sigma_2} \frac{1}{2} U_{\eta,\sigma_1} \hat{n}_{l,m,\eta} \left( \hat{n}_{l,m,\sigma_1} - \delta_{\eta,\sigma_1} \right) \] (A.48)

with \( \Phi = \phi_y = k'_y d_y \). The above Hamiltonian is an interacting spinor Hofstadter model.

Appendix B. Derivation of the generalized Heisenberg XXZ model

In the strongly interacting regime (any of \( U_{\uparrow\uparrow}, U_{\downarrow\downarrow}, U_{\uparrow\downarrow} \)) is far larger than any of \( (K, J) \), the model (A.48) with unity filling can be mapped onto a spin model, which is equivalent to a hard-core Bose–Hubbard model. Below, by using the perturbation theory for degenerated many-body quantum systems \[31\], we analytically derive an effective spin model up to second-order perturbation.

In the strongly interacting regime, one can treat the tunneling terms
\[ \hat{H}_t = \hat{H}_K + \hat{H}_J \] (B.1)
as a perturbation to the interaction term
\[ \hat{H}_0 = \sum_{l,m,\sigma} \frac{1}{2} U_{\eta,\sigma} \hat{n}_{l,m,\eta} \left( \hat{n}_{l,m,\sigma} - \delta_{\eta,\sigma} \right) \] (B.2)
where the tunneling terms are given as
\[
\begin{align*}
\hat{H}_K &= -K \sum_{l,m} \left[ \hat{T}_{l,m}^x + \hat{T}_{l,m}^y \right] \\
\hat{H}_J &= -J \sum_{l,m} \left[ \hat{T}_{l,m}^x + \hat{T}_{l,m}^y \right]
\end{align*}
\] (B.3)
with
\[
\begin{align*}
\hat{T}_{l,m}^x &= \sum_{\alpha} e^{i\alpha,x \eta^0} \hat{a}_{l+1,m,\sigma}^\dagger \hat{a}_{l,m,\sigma} \\
\hat{T}_{l,m}^y &= \sum_{\alpha} \hat{a}_{l+1,m,\sigma}^\dagger \hat{a}_{l,m,\sigma}
\end{align*}
\] (B.4)
Obviously, any Fock state is an eigenstate of \( \hat{H}_0 \). The Fock state for the system of unity filling is given as
\[ |n\rangle = |..., n_{m,\sigma}, ... \rangle = \prod_{l,m,\sigma} \frac{1}{\sqrt{n_{l,m,\sigma}!}} (\hat{a}_{l,m,\sigma}^\dagger)^{n_{l,m,\sigma}} |0\rangle \] (B.5)
where \( \sum_{l,m,\sigma} n_{l,m,\sigma} = L_x L_y = L \) (\( L_{\alpha} \) is the number of lattice sites along the \( \alpha \)-direction (\( \alpha = x \) and \( y \)), while \( L \) is the total number of sites of the whole two-dimensional lattice) and \( |0\rangle \) denotes the vacuum state. According to the eigenvalue equation \( \hat{H}_0 |n\rangle = E_n |n\rangle \), we have the eigenenergy
\[ E_n = \sum_{l,m,\sigma} \frac{1}{2} U_{\eta,\sigma} n_{l,m,\eta} \left( n_{l,m,\sigma} - \delta_{\eta,\sigma} \right) \] (B.6)
Obviously, due to there being only one atom in each lattice site, the ground-state has energy \( E_0 = 0 \) and \( 2^L \)-fold degeneracy. In the Fock basis, the ground states are expressed as
\[ |s\rangle = |..., s_{l,m}, ... \rangle = \prod_{l,m} \hat{a}_{l,m,\sigma}^\dagger |0\rangle \] (B.7)
with \( s_{l,m} \in \{ \uparrow, \downarrow \} \) and \( \hat{H}_0 |s\rangle = E_0 |s\rangle \).

The projector onto the ground-state space \( \mathcal{U}_0 \) is
\[ \hat{P}_0 = \sum_\{s\} |s\rangle \langle s| \] (B.8)
Introducing \( \mathcal{V}_0 \) as the orthogonal complement of \( \mathcal{U}_0 \), the relevant projector onto \( \mathcal{V}_0 \) is
\[ \hat{S} = - \sum_{E_n \neq 0} \frac{1}{E_n} |n\rangle \langle n| \] (B.9)
Thus the effective Hamiltonian up to second order is given as
\[ \hat{H}^{(2)} = \hat{P}_0 \hat{S} \hat{H} \hat{S} \hat{P}_0 \] (B.10)
It is easy to find that
\[
\hat{P}_0 \hat{H}_K \hat{S} \hat{H}_f \hat{P}_0 = \hat{P}_0 \hat{H}_f \hat{S} \hat{H}_f \hat{P}_0 = 0,
\]
which gives
\[
\hat{H}_{\text{eff}}^{(2)} = \hat{P}_0 \hat{H}_K \hat{S} \hat{H}_f \hat{P}_0 + \hat{P}_0 \hat{H}_f \hat{S} \hat{H}_f \hat{P}_0.
\]

Furthermore, since
\[
\begin{align*}
\hat{P}_0 \hat{S} \hat{H}_f \hat{P}_0 &= \hat{P}_0 \hat{S} \hat{H}_f \hat{P}_0,
\hat{P}_0 \hat{S} \hat{H}_f \hat{P}_0 &= \delta^\alpha_{\ell \mu} \hat{P}_0 \hat{S} \hat{H}_f \hat{P}_0,
\hat{P}_0 \hat{S} \hat{H}_f \hat{P}_0 &= \delta^\alpha_{\ell \mu} \hat{P}_0 \hat{S} \hat{H}_f \hat{P}_0,
\end{align*}
\]
for \(\alpha = x, y\), we have
\[
\hat{P}_0 \hat{H}_K \hat{S} \hat{H}_f \hat{P}_0 = K^2 \sum_{l, m} (\hat{P}_0 \hat{T}_l^\alpha \hat{S} \hat{T}_m^\alpha \hat{P}_0 + \hat{P}_0 \hat{T}_m^\alpha \hat{S} \hat{T}_l^\alpha \hat{P}_0),
\]
and
\[
\hat{P}_0 \hat{H}_f \hat{S} \hat{H}_f \hat{P}_0 = j^2 \sum_{l, m} (\hat{P}_0 \hat{T}_l^\alpha \hat{S} \hat{T}_m^\alpha \hat{P}_0 + \hat{P}_0 \hat{T}_m^\alpha \hat{S} \hat{T}_l^\alpha \hat{P}_0).
\]

This means that the effective Hamiltonian has two parts, which respectively correspond to the influences from the tunneling terms of \(x\)- and \(y\)-directions.

As the effective Hamiltonian only involves the nearest-neighbor couplings, it is sufficient to give its parameters by considering a system of two lattice sites. For tunneling along the \(x\)-direction, we take site-\(l\) as site-1 and site-\((l + 1)\) as site-2. The two-site ground states are
\[
\begin{align*}
|\uparrow, \uparrow\rangle &= \hat{a}_{\uparrow 1}^\dagger \hat{a}_{\uparrow 2}^\dagger |0\rangle, 
|\downarrow, \uparrow\rangle &= \hat{a}_{\uparrow 1}^\dagger \hat{a}_{\downarrow 2}^\dagger |0\rangle, 
|\downarrow, \downarrow\rangle &= \hat{a}_{\downarrow 1}^\dagger \hat{a}_{\downarrow 2}^\dagger |0\rangle,
\end{align*}
\]
with the eigenenergy \(E_0 = 0\). While the two-site excited states are
\[
\begin{align*}
|\uparrow\downarrow, 0\rangle &= \frac{1}{\sqrt{2}} (\hat{a}_{\uparrow 1}^\dagger)^2 |0\rangle, 
|0, \uparrow\downarrow\rangle &= \frac{1}{\sqrt{2}} (\hat{a}_{\downarrow 1}^\dagger)^2 |0\rangle, 
|\downarrow\downarrow, 0\rangle &= \hat{a}_{\downarrow 1}^\dagger \hat{a}_{\downarrow 2}^\dagger |0\rangle, 
|0, \downarrow\downarrow\rangle &= \hat{a}_{\downarrow 1}^\dagger \hat{a}_{\uparrow 2}^\dagger |0\rangle,
\end{align*}
\]
with eigenenergies \(E_{\uparrow\downarrow,0} = U_{\uparrow\uparrow}, E_{\downarrow\downarrow,0} = E_{0,\uparrow\downarrow} = U_{\downarrow\downarrow}\) and \(E_{\uparrow\downarrow,0} = E_{0,\uparrow\downarrow} = U_{\downarrow\downarrow}.\) Hence, we have the projectors
\[
\begin{align*}
\hat{P}_0 &= [\hat{a}_{\uparrow 1}^\dagger \hat{a}_{\uparrow 2}^\dagger |0\rangle \langle 0| \hat{a}_{\uparrow 1} \hat{a}_{\uparrow 2} + \hat{a}_{\downarrow 1}^\dagger \hat{a}_{\downarrow 2}^\dagger |0\rangle \langle 0| \hat{a}_{\downarrow 1} \hat{a}_{\downarrow 2}]
+ \hat{a}_{\uparrow 1}^\dagger \hat{a}_{\downarrow 2}^\dagger |0\rangle \langle 0| \hat{a}_{\uparrow 1} \hat{a}_{\downarrow 2} + \hat{a}_{\downarrow 1}^\dagger \hat{a}_{\uparrow 2}^\dagger |0\rangle \langle 0| \hat{a}_{\downarrow 1} \hat{a}_{\uparrow 2}],
\end{align*}
\]
and
\[
\begin{align*}
\hat{S} &= \frac{1}{2 U_{\uparrow\uparrow}} [\hat{a}_{\uparrow 1}^\dagger \hat{a}_{\uparrow 1} |0\rangle \langle 0| (\hat{a}_{\uparrow 1})^2] + \frac{1}{2 U_{\downarrow\downarrow}} [\hat{a}_{\downarrow 1}^\dagger \hat{a}_{\downarrow 1} |0\rangle \langle 0| (\hat{a}_{\downarrow 1})^2]
+ \frac{1}{U_{\downarrow\downarrow}} [\hat{a}_{\downarrow 1}^\dagger \hat{a}_{\uparrow 1} |0\rangle \langle 0| \hat{a}_{\downarrow 1} \hat{a}_{\uparrow 1}]
+ \frac{1}{U_{\downarrow\downarrow}} [\hat{a}_{\uparrow 1}^\dagger \hat{a}_{\downarrow 1} |0\rangle \langle 0| \hat{a}_{\uparrow 1} \hat{a}_{\downarrow 1}],
\end{align*}
\]
Inserting equations (B.17), (B.18), and (B.19) into equation (B.13), and using the bosonic commutation relations and the identity \(\hat{a}_{\alpha,j} \hat{a}_{\beta,j'}^\dagger |0\rangle = \delta_{\alpha j} \delta_{\beta j'} |0\rangle \) \((j, j' \in \{1, 2\})\), after some tedious algebra, we obtain
\[ \hat{P}_0 \hat{T}_{l,m} \hat{S}_{l,m} \hat{P}_0 = \hat{P}_0 \hat{T}_{l,m} \hat{S}_{l,m} \hat{P}_0 \]
\[ = - \left[ \frac{2}{U_{l1}} \hat{a}_{l1}^\dagger \hat{a}_{l1} \hat{a}_{l2}^\dagger \hat{a}_{l2} + \frac{2}{U_{l1}} \hat{a}_{l1}^\dagger \hat{a}_{l2} \hat{a}_{l2}^\dagger \hat{a}_{l1} \right. \\
\left. + \frac{1}{U_{l1}} (\hat{a}_{l1}^\dagger \hat{a}_{l2}^\dagger \hat{a}_{l2} \hat{a}_{l1} + \hat{a}_{l1}^\dagger \hat{a}_{l2} \hat{a}_{l2}^\dagger \hat{a}_{l1}) \right] \\
\left. + \frac{1}{U_{l1}} (e^{i2m\phi} \hat{a}_{l1}^\dagger \hat{a}_{l2} \hat{a}_{l2}^\dagger \hat{a}_{l1} + e^{-i2m\phi} \hat{a}_{l1}^\dagger \hat{a}_{l2}^\dagger \hat{a}_{l2} \hat{a}_{l1}) \right] \quad (B.20) \]

By introducing the pseudospin operators: \( \hat{S}_{l,m}^z = \hat{a}_{l,m,1}^\dagger \hat{a}_{l,m,1} - \hat{a}_{l,m,2}^\dagger \hat{a}_{l,m,2} \), \( \hat{S}_{l,m}^x = \hat{a}_{l,m,1}^\dagger \hat{a}_{l,m,2} + \hat{a}_{l,m,2}^\dagger \hat{a}_{l,m,1} \), and \( \hat{S}_{l,m}^y = \frac{1}{2} (\hat{a}_{l,m,1} - \hat{a}_{l,m,1}^\dagger) \) (we set \( \hbar = 1 \) here and after), equation (B.20) can be rewritten as
\[ \hat{P}_0 \hat{T}_{l,m} \hat{S}_{l,m} \hat{P}_0 + \hat{P}_0 \hat{T}_{l,m} \hat{S}_{l,m} \hat{P}_0 \]
\[ = - \left[ \frac{1}{U_{l1}} (e^{i2m\phi} \hat{S}_{l,m+1}^z \hat{S}_{l,m}^z + e^{-i2m\phi} \hat{S}_{l,m}^z \hat{S}_{l,m+1}^z) + 4 \left( \frac{1}{U_{l1}} + \frac{1}{U_{l1}} - \frac{1}{U_{l1}} \right) \hat{S}_{l,m}^y \right] \]
\[ + 2 \left( \frac{1}{U_{l1}} + \frac{1}{U_{l1}} - \frac{1}{U_{l1}} \right) \hat{S}_{l,m}^y \hat{S}_{l,m+1}^y + 2 \left( \frac{1}{U_{l1}} + \frac{1}{U_{l1}} + \frac{1}{U_{l1}} \right) \hat{S}_{l,m}^y \hat{S}_{l,m+1}^y \quad (B.21) \]

Extended to the lattice, that is \( 1 \rightarrow (l, m) \) and \( 2 \rightarrow (l + 1, m) \), we have
\[ \hat{P}_0 \hat{T}_{l,m} \hat{S}_{l,m} \hat{P}_0 + \hat{P}_0 \hat{T}_{l,m} \hat{S}_{l,m} \hat{P}_0 \]
\[ = - \left[ \frac{1}{U_{l1}} (e^{i2m\phi} \hat{S}_{l,m+1}^z \hat{S}_{l,m}^z + e^{-i2m\phi} \hat{S}_{l,m}^z \hat{S}_{l,m+1}^z) + 4 \left( \frac{1}{U_{l1}} + \frac{1}{U_{l1}} - \frac{1}{U_{l1}} \right) \hat{S}_{l,m}^y \right] \]
\[ + 2 \left( \frac{1}{U_{l1}} + \frac{1}{U_{l1}} - \frac{1}{U_{l1}} \right) \hat{S}_{l,m}^y \hat{S}_{l,m+1}^y + 2 \left( \frac{1}{U_{l1}} + \frac{1}{U_{l1}} + \frac{1}{U_{l1}} \right) \hat{S}_{l,m}^y \hat{S}_{l,m+1}^y \quad (B.22) \]

For tunneling along the y-direction, we take site-(l, m) as site-1 and site-(l, m + 1) as site-2. Similarly, up to second-order perturbation, we obtain
\[ \hat{P}_0 \hat{T}_{l,m} \hat{S}_{l,m} \hat{P}_0 + \hat{P}_0 \hat{T}_{l,m} \hat{S}_{l,m} \hat{P}_0 \]
\[ = - \left[ \frac{1}{U_{l1}} \left( \hat{S}_{l,m+1}^z \hat{S}_{l,m}^z + \hat{S}_{l,m}^z \hat{S}_{l,m+1}^z \right) + 4 \left( \frac{1}{U_{l1}} + \frac{1}{U_{l1}} - \frac{1}{U_{l1}} \right) \right] \hat{S}_{l,m}^y \hat{S}_{l,m+1}^y \]
\[ + 2 \left( \frac{1}{U_{l1}} + \frac{1}{U_{l1}} + \frac{1}{U_{l1}} \right) \hat{S}_{l,m}^y \hat{S}_{l,m+1}^y \quad (B.23) \]

Introducing \( J_x = 2K^2/U_{l1}, \) \( J_y = 2J^2/U_{l1}, \) \( V_x = 4K^2(1/U_{l1} + 1/U_{l1} - 1/U_{l1}), \) \( V_y = 4J^2(1/U_{l1} + 1/U_{l1} - 1/U_{l1}), \) and \( B_0 = 4(K^2 + J^2)(1/U_{l1} - 1/U_{l1}), \) from equations (B.11), (B.13), (B.14), (B.22), and (B.23), we get the effective Hamiltonian,
\[ \hat{H}^{\text{eff}} = - \sum_{l,m} \left[ J_l \hat{S}_{l,m}^+ \hat{S}_{l,m}^- + \text{h.c.} \right] + \sum_{l,m} \left[ J_l \hat{S}_{l,m+1}^+ \hat{S}_{l,m}^- + \text{h.c.} \right] \\
- \sum_{l,m} \left[ V_x \hat{S}_{l,m}^z \hat{S}_{l,m+1}^z + V_y \hat{S}_{l,m}^z \hat{S}_{l,m+1}^z \right] \right) + B_0 \sum_{l,m} \hat{S}_{l,m}^z \] 
\[ (B.24) \]

Here, we have removed a constant energy shift: \(- (K^2 + J^2)(1/U_{l1} + 1/U_{l1} - 1/U_{l1}) L_x L_y. \)

According to the Matsubara–Matsuda mapping [25]: \( |1\rangle \leftrightarrow |0\rangle, \) \( |1\rangle \leftrightarrow |1\rangle, \) \( \hat{S}_{l,m}^z \leftrightarrow |\hat{b}_{l,m}^\dagger \hat{b}_{l,m} - \hat{\varepsilon}_0 \rangle, \) the magnon excitations can be described by hard-core bosons so that the two-dimensional Heisenberg spin model (B.24) is equivalent to a two-dimensional hard-core Bose–Hubbard model subjected to a synthetic gauge field,
\[ \hat{H}_{HC} = -J \sum_{l,m} \left[ (e^{i2m\phi} \hat{b}_{l,m+1}^\dagger \hat{b}_{l,m} + \hat{b}_{l,m+1}^\dagger \hat{b}_{l,m}^\dagger) + \text{h.c.} \right] \\
- V_x \sum_{l,m} \left( \hat{b}_{l,m} \hat{\varepsilon}_{l,m+1} + \text{h.c.} \right) + B_0 \sum_{l,m} \hat{\varepsilon}_{l,m} \] 
\[ (B.25) \]
with $V_x = \Delta_x$, $V_y = \Delta_y$, and $\varepsilon_0 = \Delta_x + \Delta_y - B_0$. Here we have removed a constant energy shift $\frac{1}{4}(2B_0 - \Delta_x - \Delta_y)L_xL_y$. Since the term $\varepsilon_0\sum_{l,m} \hat{n}_{l,m}$ commutes with the other part of the Hamiltonian, it only causes a constant energy shift and thus can be removed from the Hamiltonian without changing the physics. Finally, our effective hard-core boson model obeys

$$
\hat{H} = -J_x \sum_{l,m} \left[ e^{i\varepsilon_l \phi} \hat{b}_{l+1,m}^\dagger \hat{b}_{l,m} + \lambda \hat{n}_{l,m+1} \hat{n}_{l,m} + \text{h.c.} \right] - V_x \sum_{l,m} \left( \hat{n}_{l,m} \hat{n}_{l+1,m} + \lambda \hat{n}_{l,m} \hat{n}_{l,m+1} \right) 
$$

with $\beta = \Phi/\pi$ and $\lambda = J^2/K^2$.

### Appendix C. Derivation of the effective single-particle model for two-magnon bound states

By regarding a two-magnon BS as a quasi-particle, we analytically derive an effective single-particle model via the Schrieffer–Wolff transformation [28]. As BSs appear when $|V_x/L_x| \gg 1$, one can treat the tunneling term

$$
\hat{H}_t = -J_x \sum_{l,m} \left[ e^{i\varepsilon_l \phi} \hat{b}_{l+1,m}^\dagger \hat{b}_{l,m} + \lambda \hat{n}_{l,m+1} \hat{n}_{l,m} + \text{h.c.} \right] 
$$

as a perturbation to the interaction term

$$
\hat{H}_I = -V_x \sum_{l,m} \left( \hat{n}_{l,m} \hat{n}_{l+1,m} + \lambda \hat{n}_{l,m} \hat{n}_{l,m+1} \right). 
$$

Obviously, all two-magnon Fock states $|\delta_{l,m}; l_1, m_1; l_2, m_2\rangle = \hat{b}_{l_1,m_1}^\dagger \hat{b}_{l_2,m_2}^\dagger |0\rangle$ are eigenstates of $\hat{H}_0$ with eigenvalues $E_{\delta_{l,m}; l_1, m_1}$, which are also eigenstates of $\hat{H}_0$ with eigenvalues $E_{\delta_{l,m}; l_1, m_1} = -V_x$ and $E_{\delta_{l,m}; l_1, m_1} = -\lambda V_x$ (where $\hat{H}_0|G_{l,m}^x\rangle = E_{\delta_{l,m}}^x|G_{l,m}^x\rangle$ and $\hat{H}_0|G_{l,m}^y\rangle = E_{\delta_{l,m}}^y|G_{l,m}^y\rangle$).

Using the SW transformation [28], the effective single-particle Hamiltonian up to second order reads

$$
\hat{H}_{\text{eff}}^{(2)} = \hat{h}_0 + \hat{h}_2, 
$$

$$
\hat{h}_0 = -V_x (\hat{P}_1 + \lambda \hat{P}_2), 
$$

$$
\hat{h}_2 = -\frac{1}{V_x} \left( \hat{P}_1 \hat{H}_I \hat{P}_1 + \lambda \hat{P}_2 \hat{H}_I \hat{P}_2 \right) - \frac{\lambda + 1}{2V_x} \left( \hat{P}_1 \hat{H}_I \hat{P}_1 + \hat{P}_2 \hat{H}_I \hat{P}_2 \right). 
$$

Here, the two projectors for BSs are defined as

$$
\hat{P}_1 = \sum_{l,m} |G_{l,m}^x\rangle \langle G_{l,m}^x|, 
$$

$$
\hat{P}_2 = \sum_{l,m} |G_{l,m}^y\rangle \langle G_{l,m}^y|. 
$$

For convenience, we introduce the following notation,

$$
\hat{H}_I = -J_x \sum_{l,m} \hat{n}_{l,m} + \hat{n}_{l,m}^\dagger, 
$$

$$
\hat{H}_I = -\lambda V_x \sum_{l,m} \hat{n}_{l,m} + \hat{n}_{l,m}^\dagger, 
$$

with

$$
\hat{n}_{l,m} = \hat{b}_{l,m}^\dagger \hat{b}_{l,m}, 
$$

$$
\hat{n}_{l,m} = \hat{b}_{l,m+1}^\dagger \hat{b}_{l,m}. 
$$
It is easy to find that
\[
\begin{align*}
\hat{p}_1 \hat{h}_j, \hat{h}_j \hat{p}_1 &= \hat{p}_1 \hat{h}_j, \hat{h}_j \hat{p}_1 = 0 \\
\hat{p}_2 \hat{h}_j, \hat{h}_j \hat{p}_2 &= \hat{p}_2 \hat{h}_j, \hat{h}_j \hat{p}_2 = 0 \\
\hat{p}_1 \hat{h}_j, \hat{h}_j \hat{p}_2 &= \hat{p}_1 \hat{h}_j, \hat{h}_j \hat{p}_2 = 0 \\
\hat{p}_1 \hat{h}_j, \hat{h}_j \hat{p}_1 &= \hat{p}_2 \hat{h}_j, \hat{h}_j \hat{p}_1 = 0
\end{align*}
\]
(C.9)

As \( \hat{H}_j = \hat{h}_j + \hat{h}_j \), we have
\[
\begin{align*}
\hat{p}_1 \hat{h}_j, \hat{h}_j \hat{p}_1 &= \hat{p}_1 \hat{h}_j, \hat{h}_j \hat{p}_1 + \hat{p}_1 \hat{h}_j, \hat{h}_j \hat{p}_1 \\
\hat{p}_2 \hat{h}_j, \hat{h}_j \hat{p}_2 &= \hat{p}_2 \hat{h}_j, \hat{h}_j \hat{p}_2 + \hat{p}_2 \hat{h}_j, \hat{h}_j \hat{p}_2 \\
\hat{p}_1 \hat{h}_j, \hat{h}_j \hat{p}_2 &= \hat{p}_1 \hat{h}_j, \hat{h}_j \hat{p}_2 \\
\hat{p}_2 \hat{h}_j, \hat{h}_j \hat{p}_1 &= \hat{p}_2 \hat{h}_j, \hat{h}_j \hat{p}_1
\end{align*}
\]
(C.10)

By using the hard-core bosonic commutation relations, one can obtain
\[
\begin{align*}
\hat{H}_j |G_{i,m}^{+} \rangle &= -J_x (e^{i2\pi\beta}|b_{i,m}^{+}e_{i,m}^{+}\rangle + e^{-i2\pi\beta}|b_{i,m}^{+}e_{i,m}^{+}\rangle) \\
\hat{H}_j |G_{i,m}^{-} \rangle &= -J_x (e^{i2\pi\beta}|b_{i,m}^{+}e_{i,m}^{+}\rangle + e^{-i2\pi\beta}|b_{i,m}^{+}e_{i,m}^{+}\rangle) \\
\hat{H}_j |G_{i,m}^{0} \rangle &= -\lambda J_y (\hat{b}_{i,m+1}^{+}\hat{b}_{i,m} + \hat{b}_{i,m}^{+}\hat{b}_{i,m+1}) \\
\hat{H}_j |G_{i,m}^{\infty} \rangle &= -\lambda J_y (\hat{b}_{i,m+1}^{+}\hat{b}_{i,m} + \hat{b}_{i,m}^{+}\hat{b}_{i,m+1}) \\
\hat{H}_j |G_{i,m}^{\infty} \rangle &= -\lambda J_y (\hat{b}_{i,m+1}^{+}\hat{b}_{i,m} + \hat{b}_{i,m}^{+}\hat{b}_{i,m+1}) \\
\hat{H}_j |G_{i,m}^{\infty} \rangle &= -\lambda J_y (\hat{b}_{i,m+1}^{+}\hat{b}_{i,m} + \hat{b}_{i,m}^{+}\hat{b}_{i,m+1}) \\
\end{align*}
\]
(C.11)

Therefore, we get
\[
\begin{align*}
\hat{p}_1 \hat{h}_j, \hat{h}_j \hat{p}_1 &= J_x \sum_{i,m} (e^{i2\pi\beta}|G_{i,m+1}^{\infty}\rangle \langle G_{i,m}^{\infty}| + \text{h.c.} \\
&+ 2|G_{i,m}^{\infty}\rangle \langle G_{i,m}^{\infty}|) \\
\hat{p}_1 \hat{h}_j, \hat{h}_j \hat{p}_1 &= 2\lambda J_x \sum_{i,m} (|G_{i,m+1}^{\infty}\rangle \langle G_{i,m}^{\infty}| + \text{h.c.} \\
&+ 2|G_{i,m}^{\infty}\rangle \langle G_{i,m}^{\infty}|) \\
\hat{p}_2 \hat{h}_j, \hat{h}_j \hat{p}_2 &= 2\lambda J_x \sum_{i,m} (e^{i2\pi\beta}|G_{i,m+1}^{\infty}\rangle \langle G_{i,m}^{\infty}| \\
&+ \text{h.c.} + 2|G_{i,m}^{\infty}\rangle \langle G_{i,m}^{\infty}|) \\
\hat{p}_2 \hat{h}_j, \hat{h}_j \hat{p}_2 &= \lambda J_y \sum_{i,m} (|G_{i,m+1}^{\infty}\rangle \langle G_{i,m}^{\infty}| + \text{h.c.} \\
&+ 2|G_{i,m}^{\infty}\rangle \langle G_{i,m}^{\infty}|) \\
\end{align*}
\]
(C.12)

and
\[
\hat{p}_1 \hat{h}_j, \hat{h}_j \hat{p}_2 + \hat{p}_2 \hat{h}_j, \hat{h}_j \hat{p}_1 \\
= 2\lambda J_x \cos(\pi\beta) \sum_{i,m} (e^{i2\pi\beta}|G_{i,m}^{\infty}\rangle \langle G_{i,m}^{\infty}| + \langle G_{i,m+1}^{\infty}| \langle G_{i,m}^{\infty}| + \text{h.c.}) \\
+ |G_{i,m+1}^{\infty}\rangle \langle G_{i,m}^{\infty}| + |G_{i,m+1}^{\infty}\rangle \langle G_{i,m}^{\infty}| + \text{h.c.}) \\
\]
(C.13)
Inserting equations (C.10), (C.12), (C.13) into equation (C.5), we obtain

\[
\hat{H}_\text{eff}^{(2)} = -J_{\text{eff}} \sum_{l,m} \left\{ |e^{i\pi|\hat{x}|} G_{l+1,m}^x \langle G_{l,m}^x + 2\lambda |G_{l,m+1}^y \rangle \langle G_{l,m}^y \rangle \right. \\
+ \frac{2}{\lambda} \left| e^{i\pi|\hat{x}|} \right| G_{l+1,m}^y \langle G_{l,m}^y \rangle \langle G_{l,m+1}^y \rangle + \lambda |G_{l,m+1}^y \rangle \langle G_{l,m}^y \rangle \\
+ J_{xy} | e^{i\pi|\hat{x}|} \left| e^{i\pi} \right| \left( G_{l+1,m}^{y\text{r}} \langle G_{l,m}^y \rangle + |G_{l+1,m}^y \rangle \langle G_{l,m}^y \rangle \right) \langle G_{l,m+1}^y \rangle + |h.c.| \\
+ |G_{l+1,m}^y \rangle \langle G_{l,m}^y \rangle + |G_{l+1,m}^y \rangle \langle G_{l,m}^y \rangle \right\} + \epsilon_q |G_{l,m+1}^y \rangle \langle G_{l,m}^y \rangle + \epsilon_q |G_{l,m+1}^y \rangle \langle G_{l,m}^y \rangle \right\}. \\
\]

(C.14)

Here, \( J_{\text{eff}} = J_2/V_J \), \( J_{xy} = (\lambda + 1) \cos(\pi \beta), \epsilon_s = V_x^2/J_2^2 + 2 + 4\lambda^2 \), and \( \epsilon_q = \lambda V_x^2/J_2^2 + 2\lambda + 4/\lambda \).

In order to capture the single-particle nature of the BSs, we introduce the creation operators \( \hat{A}_{l,m}^\dagger \) and \( \hat{B}_{l,m}^\dagger \) as follows: \( \hat{A}_{l,m}^\dagger \) creates a quasi-particle in the \( x \)-type BS \( |G_{l,m}^x \rangle \), while \( \hat{B}_{l,m}^\dagger \) creates a quasi-particle in the \( y \)-type BS \( |G_{l,m}^y \rangle \). That is, we define a mapping between two-magnon BSs and single-particle states: \( |G_{l,m}^x \rangle \leftrightarrow \hat{A}_{l,m}^\dagger |0\rangle \) and \( |G_{l,m}^y \rangle \leftrightarrow \hat{B}_{l,m}^\dagger |0\rangle \). Thus the effective single-particle Hamiltonian (C.14) becomes

\[
\hat{H}_\text{eff} = -J_{\text{eff}} \sum_{l,m} \left\{ |e^{i\pi|\hat{x}|} \hat{A}_{l+1,m}^\dagger \hat{A}_{l,m} + 2\lambda \hat{A}_{l+1,m}^\dagger \hat{A}_{l,m} \right. \\
+ \frac{2}{\lambda} \left| e^{i\pi|\hat{x}|} \right| \hat{B}_{l+1,m}^\dagger \hat{B}_{l,m} + \lambda \hat{B}_{l+1,m}^\dagger \hat{B}_{l,m} \\
+ J_{xy} | e^{i\pi|\hat{x}|} \left| e^{i\pi} \right| \left( \hat{A}_{l+1,m} \hat{B}_{l,m} + \hat{B}_{l+1,m}^\dagger \hat{A}_{l,m} \right) + |h.c.| \right. \\
+ |\hat{A}_{l+1,m} \rangle \langle \hat{B}_{l,m} + \hat{B}_{l+1,m}^\dagger \rangle + |\hat{B}_{l+1,m}^\dagger \rangle \left\{ \hat{A}_{l,m}^\dagger \hat{A}_{l,m} + \epsilon_q \hat{B}_{l,m}^\dagger \hat{B}_{l,m} \right\}, \\
\]

(C.15)

which describes a Hofstadter superlattice with two coupled standard Hofstadter sublattices A and B.

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