Topological invariants in two-dimensional quasicrystals

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We study the topological characterization of the energy gaps in general two-dimensional quasi-periodic systems consisting of multiple periodicities, represented by twisted two-dimensional materials. We show that every single gap is uniquely characterized by a set of integers, which quantize the area of the momentum space in units of multiple Brillouin zones defined in the redundant periodicities. These integers can be expressed as the second Chern numbers, by considering an adiabatic charge pumping under a relative slide of different periodicities, and using a formal relationship to the four-dimensional quantum Hall effect. The integers are independent of commensurability of the multiple periods, and invariant under arbitrary continuous deformations such as a relative rotation of twisted periodicities.

I. INTRODUCTION

The topological phase of matter is a fundamental concept to understand the quantum properties in crystalline solids. The topological classification relies on the existence of a gap in the energy spectrum, where the topological invariant is determined by the dependence of eigenstates below the gap on the Bloch wave number. The typical example is the integer quantum Hall effect, where the quantized Hall conductivity is expressed by the first Chern number.

The topological properties of quasicrystalline systems have also attracted much attention. Quasi-periodic systems can also have energy gaps, while the lack of the Bloch bands makes the definition of topological numbers a nontrivial problem. Several theoretical works have been devoted to topological characterization of various one-dimensional (1D) and two-dimensional (2D) quasi-periodic systems. In particular, one-dimensional quasicrystals are characterized by the adiabatic charge pumping, where the number of the transferred charge under a relative slide of a single periodic structure to the other is given by the first Chern number, in an analogous manner to the quantum Hall effect.

Recent developments in the study of 2D materials gave rise to a new class of 2D quasicrystals controlled by twist. When two atomic layers are overlaid with an arbitrary rotation angle, the periodicities of the individual layers do not generally match, and the entire system becomes quasi-periodic. A remarkable feature of these twisted 2D quasicrystals is that the electronic structure can be continuously modified by changing the twist angle or any deformations of the individual lattice structure. For instance, the twisted bilayer graphene has a highly-tunable band structure depending on the twist angle, ranging from the moiré flat bands in the small angle regime to a 12-fold rotationally symmetric quasicrystal at 30°.

Then, one can ask, what is a topological number to characterize energy gaps in a quasi-periodic system, which is invariant under a continuous structural deformation such as a relative rotation? In our previous work, we studied the energy spectrum in a quasi-periodic system of graphene sandwiched by hexagonal boron nitride (hBN) and found that each energy gap in the spectrum is uniquely characterized by a set of integers, which quantize the area of a quasi Brillouin zone in the momentum space. These integers, which we refer to as zone quantum numbers, were shown to be invariant under interlayer rotation as long as the gap remains open. It implies that there should be an underlying topological mechanism which guarantees the quantization of the momentum space area, while the actual topological expression of the zone quantum numbers is yet to be cleared.

In this paper, we consider general 2D doubly-periodic systems (i.e., 2D Hamiltonian with periodic potentials and ) which are generally incommensurate and show that six zone quantum numbers associated with every single energy gap turn out to be the second Chern numbers. The zone quantum numbers are simply defined as follows. The doubly-periodic system has the redundant reciprocal lattice vectors by taking cross product of two distinct vectors [Fig. 1(a)]. Each energy gap is then characterized by six zone quantum numbers such that the electron density below the gap is quantized as . The associated momentum area corresponds
II. ZONE QUANTUM NUMBERS

A. General formulation

We consider a doubly-periodic 2D Hamiltonian

$$H = \frac{p^2}{2m} + V^\alpha(r) + V^\beta(r), \quad (1)$$

where $V^\lambda(r)$ ($\lambda = \alpha, \beta$) is a periodic potential given by

$$V^\lambda(r) = \sum_{m_1, m_2} V_{m_1, m_2}^\lambda e^{i(m_1 b_1^\lambda + m_2 b_2^\lambda) \cdot r}, \quad (2)$$

and $b_1^\lambda, b_2^\lambda$ are its primitive reciprocal lattice vectors. The real-space lattice vectors $a_1^\lambda, a_2^\lambda$ are defined such that $a_\mu^\lambda \cdot b_\nu^\lambda = 2\pi \delta_{\mu\nu}$. It is useful to introduce serial indexes to label the four reciprocal lattice vectors as

$$(b_1, b_2, b_3, b_4) = (b_1^\alpha, b_2^\alpha, b_3^\beta, b_2^\beta). \quad (3)$$

We claim that, when the spectrum has an energy gap, the electron density below an energy gap is expressed by the second Chern numbers. By comparing the corresponding equations in the two different approaches, we find that the zone quantum numbers are equivalent to the second Chern numbers. These integers are fixed in a continuous deformation of the potential, and do not depend on the commensurability of the multiple periodicities.

The systematic characterization of energy gaps presented in this work would be applicable to general quasicrystalline systems having redundant reciprocal vectors more than the spatial dimension. The identification of the topological numbers in quasicrystalline systems bridges the fields of quasicrystal and the topological condensed matter physics.

The paper is organized as follows. In Sec. II, we present the formulation of the zone quantum numbers. We calculate the energy spectrum of a twisted double triangular potential as an example, and identify the zone quantum numbers and the quasi Brillouin zones. In Sec. III we consider the adiabatic charge pumping under a relative sliding of the double potential, and show that the pumping charge is quantized by the zone quantum numbers. In Sec. IV we present an alternative approach to describe the adiabatic charge pumping using the 4D quantum Hall effect, and find the equivalence between the zone quantum numbers and the second Chern numbers. A brief conclusion is given in Sec. V.
quantized
\[ n_e = \frac{1}{(2\pi)^2} \sum_{(i,j)} \nu_{ij} S^*_{ij} = \sum_{(i,j)} \frac{\nu_{ij}}{S_{ij}}. \] (4)

Here \( \nu_{ij} (i, j = 1, 2, 3, 4) \) are zone quantum numbers which characterize the gap, and \( (i, j) \) represents a pair of different indices. \( S^*_{ij} \) and \( S_{ij} \) are defined by
\[ S^*_{ij} = (b_i \times b_j)_z, \quad S_{ij} = (2\pi)^2/S^*_{ij}, \] (5)
where \((\cdots)_z\) represents the \( z \)-component perpendicular to the plane. \( S^*_{ij} \) is a momentum space area spanned by two distinct reciprocal lattice vectors chosen from \( b_1, b_2, b_3, b_4 \), and \( S_{ij} \) is its real-space counterpart. We have six independent areas \( S_{12}^*, S_{13}^*, S_{14}^*, S_{23}^*, S_{24}^*, S_{34}^* \) as illustrated in Fig. 1(a), and we have \( S_{ij}^* = -S_{ij}^* \) and \( S^*_{ii} = 0 \) from the definition. Accordingly, we have six zone quantum numbers \( \nu_{12}, \nu_{13}, \nu_{14}, \nu_{23}, \nu_{24}, \nu_{34} \), and we define \( \nu_{ij} = -\nu_{ji} \) and \( \nu_{ii} = 0 \) for consistency. The areas \( S^*_{ij} \) can be regarded as the projection of faces of four-dimensional hypercube onto the physical 2D plane.

The \( S_{ij} \) is the area of the parallelogram formed by the wave surfaces of \( e^{ib_i} \) and \( e^{ib_j} \), as shown in Fig. 1(b). For later convenience, we define the lattice vectors
\[ a_{ij}^1 = \frac{S_{ij}}{2\pi} (b_j \times e_z), \quad a_{ij}^2 = -\frac{S_{ij}}{2\pi} (b_i \times e_z), \] (6)
where \( e_z \) is the unit vector perpendicular to the 2D plane. \( (a_{ij}^1, a_{ij}^2) \) is the primitive lattice vector set corresponding to \( (b_{ij}^1, b_{ij}^2) \) in the momentum space, and it spans the unit cell \( S_{ij} = (a_{ij}^1 \times a_{ij}^2)_z \) as illustrated in Fig. 1(b). The lattice vectors of the potential \( \alpha \) and \( \beta \) are given by \( a_{\mu}^\alpha = a_{12}^\mu \) and \( a_{\mu}^\beta = a_{13}^\mu \).

### B. Example: Twisted triangular potentials

In our previous work\(^2\) we verified the relation Eq. 1 in a double-moiré system of graphene sandwiched by hexagonal boron nitride. There only four areas out of the six \( S_{ij}^* \)'s are independent due to the intrinsic 120° rotational symmetry, and we identified the corresponding four zone quantum numbers for the energy gaps in the spectrum. The complete set of six integers can be obtained by allowing a slight deformation to break the symmetry. In the following, we demonstrate a full identification of the six characteristic integers in a double period system Eq. 1 with twisted double triangular potential. A similar calculation with twisted square potential is presented in Appendix B.

The twisted double triangular potential is given by
\[ V^\lambda(r) = 2V_0 \sum_{\mu=1}^{3} \cos[b_\mu^\lambda \cdot (r - r_0^\lambda)], \] (7)
where \( r_0^\lambda \) is the origin of the potential \( \lambda \). The reciprocal vectors of \( \lambda = \alpha \) are given by
\[ b_1^\alpha = \frac{2\pi}{a} \left( \frac{1}{-1/\sqrt{3}} \right), \quad b_2^\alpha = \frac{2\pi}{a} \left( \frac{0}{2/\sqrt{3}} \right), \] (8)
and those of \( \beta \) are defined by
\[ b_3^\beta = R(\theta) b_\mu^\alpha, \] (9)
where \( R(\theta) \) is a 2D rotation matrix of angle \( \theta \). The corresponding primitive lattice vectors are
\[ a_1^\alpha = a_1 \left( \frac{1}{0} \right), \quad a_2^\alpha = a_2 \left( \frac{1/2}{\sqrt{3}/2} \right), \] (10)
\[ a_3^\mu = R(\theta) a_\mu^\alpha. \]

The potential profile is presented in Fig. 2 for (a) a single potential, (b) double potential with \( \theta = 7^\circ \) and (c) \( \theta = 30^\circ \). In the following, the potential amplitude (identical in \( \alpha \) and \( \beta \)) is taken as \( V_0 = 0.213\varepsilon_0 \), where \( \varepsilon_0 = \hbar^2/(2ma^2) \).

Generally, the potentials of \( \alpha \) and \( \beta \) do not have common period and hence the system does not have the global translational symmetry. Here we calculate the energy spectrum by using commensurate approximants\(^2\) which are obtained by slightly deforming the periodicity of \( \alpha \) or \( \beta \), so that the system has a finite super unit cell with an area \( S_{ij} \). The detail of the commensurate approximant method is described in Appendix A. We prepare a series of commensurate approximants to mimic the continuous rotation of the twist angle between the two potentials, and calculate the energy bands and the density of states (DOS) for all the systems. For each approximant, we average the DOS over the relative translation \( \Delta r_0 = r_0^\alpha - r_0^\beta \) to obtain a continuous spectrum as a function of the twist angle.

Figure 3(a) shows the density map of the DOS plotted against \( \theta \) and energy, where the brighter color indicates larger DOS, and the dark blue region represents the gap. The array of bars in the upper part of the figure represents the commensurate approximants considered in the calculation. Figure 3(b) is the corresponding plot with vertical axis converted to the electron density, where dots represent energy gaps with the gap width indicated by the size.
FIG. 2. Contour plots of (a) a single triangular potential, and (b) twisted double triangular potentials with $\theta = 7^\circ$ and (c) $\theta = 30^\circ$. [Eq. (7)]

![Contour plots](image)

FIG. 3. (a) Density map of the DOS plotted against $\theta$ and energy in twisted double triangular potentials. The major gaps are highlighted and labeled in the right panel. The array of bars in the upper part of the figures represents the commensurate approximants considered in the calculation. (b) Corresponding plot with vertical axis converted to the electron density, where the dot size indicates the gap width. The bottom table presents the zone quantum numbers $(\nu_{12}, \nu_{13}, \nu_{14}, \nu_{23}, \nu_{24}, \nu_{34})$ of the highlighted gaps.

For each energy gap, the zone quantum numbers $\nu_{ij}$ can be identified in the following manner. In a commensurate approximant, the momentum space area $S_{ij}^*$'s have the greatest common divisor $S_{ij}^* = (2\pi)^2/S_c$, and hence they are expressed as $S_{ij}^* = s_{ij}S_c^*$ with integers $s_{ij}$. Also, the electron density below a given band gap is quantized as $n_e = [S_c^*/(2\pi)^2]r$, where $r$ in the number of the occupied Bloch subbands. Then, Eq. (4) becomes...
the Diophantine equation \( r = \sum_{(i,j)} \nu_{ij}s_{ij} \). By considering more than six commensurate approximants sharing the same energy gap, we have the Diophantine equations as many as the number of the approximants, and we finally obtain the integers \( \nu_{ij} \) as a unique solution of the set of equations. It should be also noted that the original double triangular potential, Eq. (7), has constraints on \( S^*_{ij} \)'s such as \( S^*_{12} = S^*_{34} \) and \( S^*_{13} = S^*_{24} \) due to the high spatial symmetry, which prevents the full identification of \( \nu_{ij} \)'s. This problem is removed by including systems with the symmetry slightly broken in the set of commensurate approximants. The actual calculation of the zone quantum numbers using the commensurate approximants is presented in Appendix A.

In the bottom of Fig. 3 we present the zone quantum numbers \( (\nu_{12}, \nu_{13}, \nu_{14}, \nu_{23}, \nu_{24}, \nu_{34}) \) identified for some major gaps labelled in Fig. 3(a) and (b). The series \( M_n \) in the low twist angle regime is the moiré gaps, which has a form of

\[
M_n = n(1, 0, -1, 1, 0, 1).
\] (11)

In this region, the system is governed by a long-range moiré pattern as seen in Fig. 3(b), and the discrete levels separated by \( M_n \) can be viewed as the Bloch subbands of the moiré superlattice. The reciprocal lattice vectors for the moiré period are given by

\[
G_1^M = b_1 - b_3, \quad G_2^M = b_2 - b_4,
\] (12)

and the area of the moiré Brillouin zone becomes

\[
S^*_M = (G_1^M \times G_2^M)_z = S^*_{12} - S^*_{14} + S^*_{23} + S^*_{34}.
\] (13)

which corresponds to \((1, 0, -1, 1, 0, 1)\). Eq. (11) indicates that the momentum space area is quantized by \( S^*_M \).

In the large angle region \( \theta \gg 1^\circ \), the long-wavelength picture is no longer valid and the system cannot be effectively captured by any single periodicity. At \( \theta = 30^\circ \), in particular, the system becomes a quasicrystal with 12-fold rotational symmetry\(^{19,22}\) as shown in Fig. 2(c). Here we find that the zone quantum numbers always have the form

\[
Q_{m,n} = (m, n, 2n, -n, n, m).
\] (14)

The corresponding electronic density Eq. (4) is \( n_e = (\sqrt{3}m + 3n)/a^2 \), indicating that there are two distinct units, \( \sqrt{3}/a^2 \) and \( 3/a^2 \), to quantize the electronic spectrum.

The constraint on the zone quantum numbers Eq. (14) is explained as follows. If we define \( b'_i (i = 1, 2, 3, 4) \) by the \( 30^\circ \)-rotation of \( b_i \), we have a relation \( (b'_1, b'_2, b'_3, b'_4) = (b_3, b_4, b_1 + b_2, -b_1). \) The associated areas \( S^*_{ij} \)'s can be expressed by the old areas as \( S^*_{ij} = S^*_{34}, S^*_{13} = -S^*_{13} - S^*_{23}, \) etc. When the system is invariant under the \( 30^\circ \)-rotation, we should have \( \sum_{(i,j)} \nu_{ij}S^*_{ij} = \sum_{(i,j)} \nu_{ij}S^*_{ij} \) with the identical \( \nu_{ij} \). By using the relationship between \( S^*_{ij} \) and \( S^*_{ij} \), we obtain constraints for \( \nu_{ij} \), and finally find Eq. (14).

Other gaps are just labelled as \( A, B, C \cdots \) in Fig. 3. We see that the zone quantum numbers of any gaps definitely come in a form of \((m, n, r, n - r, n, m)\). This is explained by the coexistence of the \( 120^\circ \) rotational symmetry which requires the form of \((m, n, r, n - r, n, m')\), and the reflection symmetry with respect to the in-plane axis between \( b_1 \) and \( b_3 \) which requires \((m, n, r, n - r, m', m)\). The constraints on the zone quantum numbers are proved by a similar argument to the 12-fold case.

In our previous work\(^{53}\), we obtained only four zone quantum numbers in hBN/graphene/hBN systems because we only considered strictly \( 120^\circ \)-symmetric commensurate approximants. There the unit areas have relationship \( S^*_{24} = S^*_{13} \) and \( S^*_{23} = -S^*_{14} \), so that \( \sum_{(i,j)} \nu_{ij}S^*_{ij} \) is reduced to \( m_1S^*_{12} + m_3S^*_{14} + m_4S^*_{14} \) with \((m_1, m_2, m_3, m_4) = (\nu_{12}, \nu_{13}, \nu_{14} - \nu_{13} - \nu_{14}, \nu_{14}) \). The four integers defined in Ref. 53. Recalling that \( \nu_{ij} \) must have the form \((m, n, r, n - r, n, m')\) in \( 120^\circ \)-symmetry, we can restore the complete six numbers \( \nu_{ij} \) as \((m_1, 2m_2 - m_4, m_3 + m_4, m_3 - 2m_4, 2m_3 - m_4, m_2)\). The numbers are found to be integers for all the gaps identified in Ref. 53.

C. Quasi Brillouin zones

The area \( \sum_{(i,j)} \nu_{ij}S^*_{ij} \) can be associated with a geometric object in the momentum space referred to as the quasi Brillouin zone (qBZ). The boundary qBZ for a given gap is defined as a set of \( k \)-points on the original free-electron band, at which the gap starts to open in the infinitesimal potential limit\(^{53}\). Generally, the qBZ is a polygon composed of multiple segments of Bragg planes, which are the perpendicular bisectors of composite reciprocal lattice vectors \( G = m_1b_1 + m_2b_2 + m_3b_3 + m_4b_4 \).

Let us consider the twisted triangular potential considered in the previous section. The qBZ for the moiré gap \( M_n \) is found to be just \( n \)-th Brillouin zone defined by the moiré reciprocal vectors \( G^M_1 \) and \( G^M_2 \) [Eq. (12)]. In general twist angles, however, the qBZ does not coincide with any Brillouin zone of a periodic system. We show the qBZs of the gap \( Q_{-1,1} \) and \( Q_{-3,2} \) at \( \theta = 30^\circ \) in the leftmost panels of Fig.
as shown Fig. 4(b). The area cell in the reciprocal lattice of expressed by \( S(p,q) \) primitive vectors the first and second Brillouin zones defined by the obtained in the previous section.

With the zone quantum numbers (\( -Q, h \)) treated in the right two panels. For instance, the area can be easily calculated by the decomposition illustrated in each row in Fig. 4(a) and (b), respectively. The areas of these qBZs in each row illustrate the decomposition of the qBZ into the primitive Brillouin zones.

Similarly, the area of the qBZ for gap \( Q_{-3,2} \) is expressed by \( S^\ast(Q_{-3,2}) = p_1 + p_2 + p_3 - 2q_1 - q_2 \) as shown Fig. 4(b). The area \( p_1 \) is the Wigner-Seitz cell in the reciprocal lattice of \( b_1 \) and \( b_3 \), and hence \( p_1 = S_{13}^\ast \). The \( q_1 \) (hexagon) and \( q_2 \) (six triangles) are the first and second Brillouin zones defined by the primitive vectors \( b_3 - b_1 \) and \( b_2 - b_4 \), and therefore \( q_1 = q_2 = [(b_1 - b_3) \times (b_2 - b_4)]_z = S_{12}^\ast + S_{24}^\ast - S_{14}^\ast + S_{23}^\ast \). As a result, the area \( S^\ast(Q_{-3,2}) \) becomes (-3, 2, 4, -2, 2, -3).

At 30°, we have the symmetry constraints such as \( g_1 = g_2 = g_3 \) and one might think the decomposition of the qBZ area into \( S_{ij}^\ast \)'s is not unique. However, the area quantization with the same \( \nu_{ij} \) strictly holds when the potential is deformed to break the symmetry, and this guarantees a uniqueness of the decomposition.

III. ADIABATIC CHARGE PUMPING

Here we show that the zone quantum numbers introduced in the previous section characterize the adiabatic charge pumping under the relative sliding of the doubly periodic potential.
A. 1D systems

We first consider a doubly-periodic 1D Hamiltonian

\[ H = \frac{p^2}{2m} + V_1(x) + V_2(x), \]  

(15)

where \( V_i(x) = \sum_{m} V_{i,m} e^{imbx}(i = 1, 2) \) is a periodic potential with the period of \( a_i = 2\pi/b_i \). Now we consider a cyclic process where one of the periodic potential \( V_i(x) \) is adiabatically translated by its period \( a_i \), with the other fixed. The translated potential is expressed as

\[ V_i(x - \frac{\phi_1}{2\pi} a_i) = \sum_{m} V_{i,m} e^{im(b_i x - \phi_i)}, \]  

(16)

where an increase of \( \phi_i \) from 0 to \( 2\pi \) gives a unit slide of \( V_i(x) \) by distance \( a_i \).

We define \( \Delta P_i \) by the change of the electric polarization during a unit slide. In 1D, the \( \Delta P_i \) has a dimension of the electronic density (number of electrons per a unit length) times length, which is dimensionless. Note that we exclude the electric charge \(-e\) in the definition of the polarization. Here we claim the following: When the Fermi energy is in a gap, the corresponding change of \( V_i \), and the electron density below the gap, \( n_e \), are related by

\[ \Delta P_i = 2\pi \frac{\partial n_e}{\partial b_i}. \]  

(17)

Eq. (17) can be proved by the following consideration. Let us consider an adiabatic process where the wavenumber \( b_i \) is slightly changed to \( b_i + \delta b_i \). As illustrated in Fig. 5, the corresponding change of \( V_i(x) \) at a point far from the origin (\( |x| \gg a_i \)) can be viewed as a parallel translation of the fixed potential \( V_i(x) \). Considering the phase factor \( b_i x - \phi_i \) in Eq. (16), the change of \( b_i \) to \( b_i + \delta b_i \) can be absorbed to the change of \( \phi_i \) by \( \delta \phi_i = -\delta b_i x \), and this gives the phase shift in the effective translation at \( x \). Since this process amounts to \( n = \delta \phi_i/(2\pi) \) cycles of a unit translation, the number of electrons passing through the point \( x \) is given by \( n\Delta P_i = -\Delta P_i \delta b_i x/(2\pi) \). Due to the continuity of the electric charge, it must be equal to the change of the number of the electrons in a region from 0 to \( x \). This leads to a relation

\[ -\Delta P_i \delta b_i x/(2\pi) = -x \delta n_e, \]  

and we obtain Eq. (17).

In the doubly-periodic system given by Eq. (15), every gap in the spectrum is characterized by a pair of integers \( m_1 \) and \( m_2 \), such that the electron density below the gap is given by

\[ n_e = \frac{1}{2\pi} (m_1 b_1 + m_2 b_2) = \frac{m_1}{a_1} + \frac{m_2}{a_2}, \]  

(18)

By using Eq. (17), we conclude \( \Delta P_i = m_i \), i.e., \( m_i \) electrons passed through any cross section of the system. The integers \( m_1 \) and \( m_2 \) coincide with the first Chern numbers \( \lambda_1, \lambda_2 \), as presented in Appendix A.

B. 2D systems

The same argument is available for a doubly-periodic 2D Hamiltonian, Eq. (1). We consider an adiabatic translation of the periodic potential \( V^\lambda \) (\( \lambda = \alpha \) or \( \beta \)) by \( a_\mu^\lambda \), and calculate the change of the electric polarization during the process. A parallel translation of \( V^\lambda(r) \) is expressed as

\[ V^\lambda (r - \frac{\phi_\lambda_1}{2\pi} a_\mu^\lambda - \frac{\phi_\lambda_2}{2\pi} b_\nu^\lambda) = \sum_{m_1, m_2} V_{m_1,m_2}^\lambda e^{im_1 (b_\mu^\lambda \cdot r - \phi_\lambda_1) + im_2 (b_\nu^\lambda \cdot r - \phi_\lambda_2)} \]  

(19)

where we used \( a_\mu^\lambda \cdot b_\nu^\lambda = 2\pi \delta_{\mu\nu} \). An increase of \( \phi_\lambda^\mu \) from 0 to \( 2\pi \) gives a unit translation of the potential \( V^\lambda \) by \( a_\mu^\lambda \).

The situation can be systematically described by a generalized Hamiltonian \( H = p^2/(2m) + V \) with

\[ V(r; \phi_1, \cdots, \phi_N) = \sum_{m_1, \cdots, m_N} V_{m_1,\cdots,m_N} e^{i\sum_{i=1}^N m_i (b_i \cdot r - \phi_i)}. \]  

(20)

The current double-period system corresponds to \( N = 4 \), where \( b_1, \cdots, b_4 \) are given by Eq. (3), and

\[ (\phi_1, \phi_2, \phi_3, \phi_4) = (\phi_1^\alpha, \phi_2^\alpha, \phi_3^\beta, \phi_4^\beta). \]  

(21)

We consider a cyclic process where \( \phi_1 \) of a certain \( i \) is adiabatically increased from 0 to \( 2\pi \). When the
Fermi energy is in a gap, we can show that the change of the electric polarization during the process is

$$\Delta \mathbf{P}_i = 2\pi \frac{\partial n_{e_i}}{\partial \mathbf{b}_i},$$

(22)

which is the 2D version of Eq. (17). Now $\Delta \mathbf{P}_i$ has a dimension of the electronic density (number of electrons per a unit area) times length.

Eq. (22) is derived as follows. Let us consider the change of the potential $V(\mathbf{r})$ when $\mathbf{b}_i$ is changed to $\mathbf{b}_i + \delta \mathbf{b}_i$. In a similar manner to 1D case, the change at a point far from the origin ($|\mathbf{r}| \gg 2\pi/|\mathbf{b}_i|$) is equivalent to a parallel translation of $-\delta \mathbf{b}_i \cdot \mathbf{r}$, noting the phase factor $\mathbf{b}_i \cdot \mathbf{r} - \phi_i$ in Eq. (20). This causes a polarization change by

$$\Delta \mathbf{P}_i \delta \phi_i / (2\pi) = \Delta \mathbf{P}_i (\delta \mathbf{b}_i \cdot \mathbf{r}) / (2\pi)$$

at the point $\mathbf{r}$. The number of electrons passing through a line segment from $\mathbf{r}$ to $\mathbf{r} + d\mathbf{r}$ is given by

$$dN_e = [(d\mathbf{r} \times \mathbf{e}_z) \cdot \Delta \mathbf{P}_i (\delta \mathbf{b}_i \cdot \mathbf{r})] / (2\pi).$$

(23)

Now we consider a large closed path $C$ on the 2D plane, and let $N_e$ the number of electrons inside $C$. When $\mathbf{b}_i$ is changed to $\mathbf{b}_i + \delta \mathbf{b}_i$, the change of the $N_e$ is calculated by integrating Eq. (23) along the path, to obtain

$$\delta N_e = \oint_C dN_e = \frac{1}{2\pi} \oint_C [(d\mathbf{r} \times \mathbf{e}_z) \cdot \Delta \mathbf{P}_i (\delta \mathbf{b}_i \cdot \mathbf{r})]$$

= \frac{S}{2\pi} \Delta \mathbf{P}_i \cdot \delta \mathbf{b}_i$$

(24)

where $S$ is the area of the region enclosed by $C$ and we used the relationship $\oint_C (d\mathbf{r} \times \mathbf{e}_z) \mu_{\nu} = S \delta_{\mu\nu}$ in 2D. Since $n_e = N_e/S$, we end up with Eq. (22).

Alternatively, Eq. (22) can also be derived in the infinitesimal potential limit, by integrating the Berry curvature on the boundary of the quasi Brillouin zone. The detailed argument is presented in Appendix C.

In a 2D doubly-periodic system, the electron density below an energy gap is quantized by Eq. (4), as argued in the previous section. By applying the formula Eq. (22) to Eq. (4), the charge pumping $\Delta \mathbf{P}_i$ is explicitly calculated as

$$\Delta \mathbf{P}_i = \frac{1}{2\pi} \sum_{(k,j)} \nu_{kj}^* S_{kj}^* \frac{\partial \mathbf{b}_i}{\partial \mathbf{b}_i},$$

(25)

where we used $S_{kj}^* = (\mathbf{b}_i \times \mathbf{b}_j) \cdot \mathbf{e}_z = (\mathbf{b}_j \times \mathbf{e}_z) \cdot \mathbf{b}_i$.

By using the real space lattice vectors Eq. (6), Eq. (25) can also be written as

$$\Delta \mathbf{P}_i = \sum_j \frac{\nu_{ij}}{S_{ij}} \mathbf{a}_{ij}.$$

(26)

The physical interpretation of Eq. (26) is as follows. Eq. (4) states that $\nu_{ij}$ electrons reside in each unit area of $S_{ij}$. When $\phi_1$ is changed from 0 to $2\pi$ (i.e., $V^\alpha$ is slid by $\mathbf{a}_i^\alpha$), for instance, the wave surface of $\mathbf{b}_1$ is slid by its single period, resulting in shifts of the unit areas $S_{12}, S_{13}, S_{14}$ by $\mathbf{a}_{12}^\alpha, \mathbf{a}_{13}^\alpha, \mathbf{a}_{14}^\alpha$, respectively [See, Fig. 1(b)]. For each of $j = 2, 3, 4$, the electron density of $\nu_{ij}/S_{ij}$ is transferred by $\mathbf{a}_{ij}^\alpha$, resulting in a polarization change by

$$\Delta \mathbf{P}_i = \sum_{j=2,3,4} \nu_{ij}/S_{1j} \mathbf{a}_{ij}.$$

C. Example: Twisted triangular potentials

As an example, we consider the adiabatic pumping in the twisted triangular potential in Sec. IIIB. For the moiré gap $M_n = n(1, 0, -1, 1, 0, 1)$ [Eq. (11)], Eq. (25) immediately leads to equations

$$\Delta \mathbf{P}_1 = \frac{n}{2\pi} (\mathbf{b}_2 - \mathbf{b}_4) \times \mathbf{e}_z = \frac{n}{S_{12}^M} \mathbf{L}_1^M,$$

$$\Delta \mathbf{P}_2 = \frac{n}{2\pi} (\mathbf{b}_1 - \mathbf{b}_3) \times \mathbf{e}_z = \frac{n}{S_{13}^M} \mathbf{L}_2^M,$$

$$\Delta \mathbf{P}_3 = \frac{n}{2\pi} (\mathbf{b}_2 - \mathbf{b}_4) \times \mathbf{e}_z = \frac{n}{S_{14}^M} \mathbf{L}_1^M,$$

$$\Delta \mathbf{P}_4 = \frac{n}{2\pi} (\mathbf{b}_1 - \mathbf{b}_3) \times \mathbf{e}_z = \frac{n}{S_{12}^M} \mathbf{L}_2^M,$$

(27)

where $\mathbf{L}_i^M$ is the moiré lattice vector defined by

$$\mathbf{L}_i^M = \frac{S_{12}^M}{2\pi} (\mathbf{G}_i^M \times \mathbf{e}_z), \quad \mathbf{L}_2^M = \frac{S_{12}^M}{2\pi} (\mathbf{G}_1^M \times \mathbf{e}_z),$$

(28)

and we used Eq. (12). This indicates that, when the potential $\alpha(\beta)$ is slid by its unit vector $\mathbf{a}_i^\alpha(\mathbf{a}_i^\beta)$, then $n$ electrons per the moiré unit cell are pumped by a moiré unit vector $n \mathbf{L}_i^M \times (-n \mathbf{L}_i^M)$. The result coincides with the adiabatic moiré pumping in the previous works.

The argument is also applicable to the quasicrystal gaps at $\theta = 30^\circ$. Here the zone quantum numbers take the form $Q_{m,n} = (m, n, 2n, -n, n, m)$ [Eq. (14)]. For $\Delta \mathbf{P}_1$, for instance, Eq. (25) gives

$$\Delta \mathbf{P}_1 = \frac{1}{2\pi} (mb_2 + nb_3 + 2nb_4) \times \mathbf{e}_z$$

= \frac{1}{L} (m + \sqrt{3}n) \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} = \frac{n_e}{2} \mathbf{a}_1^\alpha.$$
In the last equation, we used Eq. (10) and note that the electronic density [Eq. (4)] is \( n_e = (\sqrt{3}m + 3n)/L^2 \) at \( \theta = 30^\circ \). By similar calculations, we have a set of equations independent of \( m \) and \( n \),

\[
\begin{align*}
\Delta P_1 &= \frac{n_e}{2} a_1^\alpha, \\
\Delta P_2 &= \frac{n_e}{2} a_1^\beta, \\
\Delta P_3 &= \frac{n_e}{2} a_1^\gamma, \\
\Delta P_4 &= \frac{n_e}{2} a_1^\delta.
\end{align*}
\]

From the definition, \( \Delta P_1 \) and \( \Delta P_2 \) (\( \Delta P_3 \) and \( \Delta P_4 \)) represent the polarization changes when the potential \( \alpha \) (\( \beta \)) is translated by \( a_1^\alpha \) and \( a_1^\beta \) (\( a_1^\gamma \) and \( a_1^\delta \)), respectively. Eq. (30) shows that, in any sliding processes, the transfer of the electric charge is always parallel to the potential sliding direction (regardless of which potential we move), and that the amount of the charge pumping is equivalent to the movement of the half of the total electric charge by the sliding vector.

**IV. 4D QUANTUM HALL EFFECT AND THE SECOND CHERN NUMBERS**

In the following, we describe the adiabatic pumping argued in the previous section in an alternative approach using the dimensional reduction of the four-dimensional (4D) quantum Hall effect (QHE), and demonstrate that the zone quantum number \( \nu_{ij} \) coincides with the second Chern number.

We first consider the 3D QHE as a simple example. Let us consider an infinite stack of 2D free-electron systems as illustrated Fig. 6, which is continuous in \( x \) and \( y \) directions and discrete in \( z \) direction with lattice spacing \( a_z \). For \( z \)-direction, we assume the nearest-neighbor tight-binding coupling \( t_z \) between the adjacent layers. We apply a magnetic field \( B_{\mu \nu} = \partial_{\mu} A_\nu - \partial_{\nu} A_\mu \). Here we assume a uniform, in-plane field \( B = (B_{yx}, B_{zx}, 0) \), and set the vector potential as \( A = (0, 0, A_z) \) with \( A_z = B_{zz} x + B_{yz} y \) (note \( B_{zz} = -B_{zx} \)). The motion of an electron is described by the Schrödinger equation,

\[
\frac{p^2}{2m} \psi(x, y, z) - t_z \left[ e^{i\pi A_z a_z} \psi(x, y, z + a_z) + e^{-i\pi A_z a_z} \psi(x, y, z - a_z) \right] = E \Psi(x, y, z),
\]

where \( p = -i\hbar(\partial_x, \partial_y) \) is the in-plane momentum. Since the Hamiltonian is periodic in \( z \), the wavefunction can be factorized as \( \Psi(x, y, z) = \psi(x, y) e^{ik_z z} \), and then Eq. (31) is reduced to a 2D Schrödinger equation,

\[
\frac{p^2}{2m} \psi - 2t_z \cos(b \cdot x + \phi_z) \psi = E \psi,
\]

where \( b = (ea_z/h)(B_{xx}, B_{yx}) \), \( x = (x, y) \) and \( \phi_z = k_z a_z \). This is a 2D system with a single sinusoidal potential with the wave number \( b \). The phase factor \( \phi_z \) corresponds to the wavenumber in \( z \) direction.

The extension of higher dimensions is straightforward. We consider a six-dimensional (6D) system in \( x, y, z_1, z_2, z_3, z_4 \) space, which is continuous in \( x \) and \( y \) directions and discrete in \( z_i \) \((i = 1, 2, 3, 4) \) direction. We apply a uniform magnetic field \( B_{yi} \) and \( B_{ix} = -B_{xi} \) on \( yz_i \)-plane and \( z_i \)-plane, respectively, and take the vector potential \( A = \sum_{i=1}^{4} (B_{yi} x + B_{xi} y) \mathbf{e}_i \) where \( \mathbf{e}_i \) is the unit vector in \( z_i \) direction. As the Hamiltonian is periodic in any \( z_i \)’s, the wavefunction can be written as \( \Psi(x, y, z_1, z_2, z_3, z_4) = \psi(x, y) e^{i\sum_{k=1}^{4} k_i z_i} \), where \( k_i \) is the Bloch wavenumber defined in \( \pi/a_i < k_i \leq \pi/a_i \). The 6D Schrödinger equation is reduced to \( (x, y) \) space as

\[
\frac{p^2}{2m} \psi - \sum_{i=1}^{4} 2t_i \cos(b_i \cdot x + \phi_i) \psi = E \psi,
\]

where

\[
b_i = \frac{ea_i}{\hbar}(B_{xi}, B_{yi}), \quad \phi_i = k_i a_i.
\]

This is equivalent to the double-period 2D system considered in this paper. The higher harmonic terms in \( b_i \) can be incorporated by assuming the further layer hopping in \( z \) direction.

The electromagnetic response of the system is characterized by the second Chern number. Let us consider a commensurate approximant where the periodicities of \( b_i \) \((i = 1, 2, 3, 4) \) have a common super unit cell, and define the Bloch wavenumber \( (k_x, k_y) \) in the corresponding super Brillouin zone.
The Bloch Hamiltonian for the 4D system is written as $H(k_x, k_y, k_1, k_2, k_3)$. We consider the 4D subspace $k_\mu = (k_x, k_y, k_1, k_2)$ by choosing two indexes $i, j$ from 1 to 4, with the rest two wavenumbers fixed. When the spectrum of 4D Hamiltonian $H(k_x, k_y, k_1, k_2)$ is gapped, the second Chern number for the gap is defined as\cite{21}:

$$C^{(2)}_{ij} = \frac{1}{2\pi^2} \int_{BZ} d^4k \epsilon^{\mu\nu\lambda\rho} \text{Tr}[\mathcal{F}_{\mu\nu} \mathcal{F}_{\lambda\rho}] \in \mathbb{Z}. \quad (35)$$

Here BZ stands for the 4D Brillouin zone (a 4D torus), $\epsilon^{\mu\nu\lambda\rho}$ is the antisymmetric tensor of rank 4 and $\mathcal{F}_{\mu\nu}$ is a matrix defined by

$$\mathcal{F}_{\mu\nu} = \partial_{\mu} A_{\nu} - \partial_{\nu} A_{\mu} + i[A_{\mu}, A_{\nu}]^\alpha\beta,$$

$$A_{\mu}^\alpha (k) = -i(\alpha, k|\partial|/\beta, k), \quad (36)$$

where $\partial_{\mu} = \partial/\partial k_{\mu}$, $|\alpha, k\rangle$ is the eigenstates of the $\alpha$-th band, and the indexes $\alpha$ and $\beta$ run over all the bands below the gap. It is alternatively expressed as\cite{21}

$$C^{(2)}_{ij} = \frac{1}{8\pi^2} \int_{BZ} d^4k \epsilon^{\mu\nu\lambda\rho} \text{Tr} \left[ P \frac{\partial P}{\partial k_{\mu}} \frac{\partial P}{\partial k_{\nu}} E \frac{\partial P}{\partial k_{\lambda}} \frac{\partial P}{\partial k_{\rho}} \right] \quad (37)$$

where $P(k) = \sum_{\alpha \in \text{occ}} |\alpha, k\rangle \langle \alpha, k|$ is the projection operator to the eigenstates below the gap. Note that we have six second Chern numbers depending on the choice of $i, j$ ($i \neq j$) from 1, 2, 3, 4.

When the Fermi energy is in the gap, the electro-magnetic response of the 4D system is given by\cite{21}\cite{22}\cite{27}

$$j^{(4D)}_{\mu} = \frac{e^3}{\hbar^2} C^{(2)}_{ij} \epsilon^{\mu\nu\lambda\rho} B_{\nu\lambda} E_{\delta}, \quad (38)$$

where $j^{(4D)}_{\mu}$ is the electric current density in the 4D space. If a weak electric field $E_i$ is applied to the system, the wavenumber $k_i$ is adiabatically changed to $k_i + (e/\hbar) A_i(t)$, where $E_i = -\partial A_i/\partial t$. When we consider a cyclic process where $\phi_i = k_i a_i$ is changed from 0 to $2\pi$ in a time period $T$, the corresponding electric field should be

$$E_i = -\frac{e}{ea_i} \frac{1}{T}. \quad (39)$$

According to Eq. (38), $E_i$ induces an electric current

$$(j_x, j_y)^{(4D)} = (e^3/\hbar^2) C^{(2)}_{ij} (B_2, B_3) E_i.$$  

The corresponding 2D current density per a single layer is given by

$$j^{(2D)}_{\mu} = j^{(4D)}_{\mu} a_i a_j,$$

$$j_x^{(2D)} = \frac{-e}{2\pi} C^{(2)}_{ij} (b_{j,y}, -b_{j,x}) \frac{1}{T}, \quad (40)$$

where we used Eqs. (34) and (39). Total polarization change in the process ($\phi_i : 0 \to 2\pi$) is

$$\Delta P_i = \frac{-1}{2\pi} \sum_j C^{(2)}_{ij} (b_j \times e_z). \quad (41)$$

We notice that Eq. (41) has the exactly the same form as Eq. (25). By comparing the two equations, we immediately find

$$\nu_{ij} = -C^{(2)}_{ij}, \quad (42)$$

i.e., the zone quantum numbers turned out to be the second Chern numbers.

By using Eq. (37), we numerically calculated $C^{(2)}_{ij}$ for some of commensurate approximants in the twisted triangular potential series considered in Sec. \cite{11}, and confirmed the agreement with $-\nu_{ij}$. Since Eq. (37) includes the integral on the Brillouin zone of the commensurate approximant, one might think that $C^{(2)}_{ij}$ explicitly depends on the Brillouin zone size (inverse of the commensurate unit cell size), which is rather arbitrary as seen in Appendix A. But in reality, the integrand $\text{Tr} [\cdots]$ itself is proportional to the number of the subbands below the gap (proportional to the unit cell size), and this cancels with the Brillouin zone integral, giving the invariant integers independent of the commensurate period.

V. CONCLUSION

We have shown that energy gaps in two-dimensional double-periodic systems can be uniquely labelled by six second Chern numbers. Physically, these numbers can be interpreted as zone quantum numbers, which quantize the momentum space in units of the six fundamental Brillouin zones defined in the redundant periodicities. At the same time, the zone quantum numbers also describe the quantized charge pumping under a relative slide of different periodic potentials. By considering a mapping of the 2D charge pumping to the fictitious 4D quantum Hall effect, we found the zone quantum numbers are equivalent to the second Chern numbers.

The topological characterization of energy gaps presented in this work is applicable to any quasi-periodic systems having redundant reciprocal vectors more than the spatial dimension. In a twisted multi-layer system composed on $n$ layers, for instance, $2n$ reciprocal vectors define $n(2n - 1)$ independent Brillouin zones, so that there should be $n(2n - 1)$ zone
quantum numbers. The Penrose tiling has 5 reciprocal lattice vectors, giving the 10 quantum numbers. The extension to 3D quasicrystal should also be possible. Lastly, non-zero quantum numbers for adiabatic pumping generally implies the existence of the edge localized states. The study of the edge states in general quasiperiodic systems in terms of the zone quantum numbers would also be intriguing.

Appendix A: Commensurate approximant method

We describe the commensurate approximant method to calculate the band structures and the zone quantum numbers in the double-period system. In an incommensurate case, we always have lattice points of the two periodic potentials which happen to be very close to each other. The situation is expressed as

\[ p_1 a_1^\alpha + p_2 a_2^\alpha = p_3 a_1^\beta + p_4 a_2^\beta + \Delta L, \]  

(A1)

where \( p_i \) (\( i = 1, 2, 3, 4 \)) are integers and \( \Delta L \) is the difference.

A commensurate approximant can be obtained by choosing two such nearly-commensurate points [with integers \((p_1, p_2, p_3, p_4)\) and \((q_1, q_2, q_3, q_4)\)], and deforming the potential \( \beta \) such that \( \Delta L \) becomes zero. The two points then become the exact primitive lattice vectors of the commensurate approximant,

\[ \begin{pmatrix} a_1^\alpha \\ a_2^\alpha \end{pmatrix} = \begin{pmatrix} p_1 & p_2 \\ q_1 & q_2 \end{pmatrix} \begin{pmatrix} a_1^\beta \\ a_2^\beta \end{pmatrix} = \begin{pmatrix} p_3 & p_4 \\ q_3 & q_4 \end{pmatrix} \begin{pmatrix} a_1^\beta \\ a_2^\beta \end{pmatrix}. \]  

(A2)

Correspondingly, the reciprocal superlattice vectors \( b_1^\dagger, b_2^\dagger \) are given by

\[ \begin{pmatrix} b_1^\dagger \\ b_2^\dagger \end{pmatrix} = \left[ \begin{pmatrix} p_1 & p_2 \\ q_1 & q_2 \end{pmatrix} \right]^T \begin{pmatrix} b_1^\alpha \\ b_2^\alpha \end{pmatrix} = \left[ \begin{pmatrix} p_3 & p_4 \\ q_3 & q_4 \end{pmatrix} \right]^T \begin{pmatrix} b_1^\beta \\ b_2^\beta \end{pmatrix}. \]  

(A3)

where \( T \) stands for the matrix transpose. \( a_1^\mu \) and \( b_1^\mu \) are related by

\[ a_1^\mu = \frac{S_c}{2\pi} (b_2^\mu \times e_z), \quad a_2^\mu = -\frac{S_c}{2\pi} (b_1^\mu \times e_z), \]  

(A4)

where \( S_c = (a_1^\alpha \times a_2^\alpha)_z \) is the unit area of the commensurate approximant.

By using the serial notation Eq. (3), Eq. (A3) can simply be written as

\[ b_i = p_i b_1^\mu + q_i b_2^\mu. \]  

(A5)

Accordingly, the unit areas Eq. (5) become

\[ S_{ij}^* = (p_i q_j - p_j q_i) S_c^*, \]  

(A6)

where \( S_{ij}^* = (b_1^\mu \times b_2^\mu)_z = (2\pi)^2 / S_c \) is the area of the first Brillouin zone of the commensurate approximant. Eq. (4) becomes the Diophantine equation,

\[ r = \sum_{(i,j)} \nu_{ij} (p_i q_j - p_j q_i), \]  

(A7)

where \( r \equiv n_c / [S_c^*(2\pi)^2] \) is for the number of the bands below the gap.

In determination of the zone quantum numbers \( \nu_{ij} \), we consider a series of commensurate approximants near the target system, and solve a set of Diophantine equations Eq. (A7) for all the approximants. As an example, we show in Fig. 7 the band structures of six commensurate approximants near the target system, and solve a set of Diophantine equations Eq. (A7) for all the approximants. As an example, we show in Fig. 7 the band structures of six commensurate approximants (a) to (f) for the double triangular potential near \( \theta = 30^\circ \) [see, Fig. 3], which are specified by \((p_1, p_2, p_3, q_1, q_2, q_3, q_4)\) in Table I. The Brillouin zone path is taken as \((\Gamma, A, C, B, \Gamma) \equiv (0, b_1^\dagger / 2, (b_1^\dagger + b_2^\dagger)/2, b_2^\dagger/2, 0)\). Table I also shows the number of the occupied bands \( r \) for some major gaps \( Q_{m,n} \). The six systems have very close potential profiles and similar spectral structures, while it have completely different sizes of the commensurate unit cells and thus different numbers of bands below the same gap. For the largest gap \( Q_{-1,1} \), for instance, the number of the bands are \( r = 142, 254, 1710, 265, 1978, 724 \) for the six systems, and accordingly we have six independent equations of Eq. (A7) with six unknown variables \( \nu_{ij} \). By solving the set of the equations, we find \( \nu_{ij} = (-1, 1, 2, -1, 1, -1) \) as a unique solution. All other approximants sharing the same gap have the same solution of \( \nu_{ij} \).

The formula of quantum pumping Eq. (25) can also be transformed to the commensurate version. By using Eq. (A5), Eq. (25) is written as

\[ \Delta P_i = \frac{1}{2\pi} \sum_{j \neq i} \nu_{ij} [p_j (b_1^\dagger \times e_z) + q_j (b_2^\dagger \times e_z)]. \]  

(A8)

By using Eq. (A4), it is reduced to

\[ \Delta P_i = \frac{1}{S_c} (C_1 a_1^\mu + C_2 a_2^\mu), \]  

(A9)
The integers in gaps indicate the number of the bands below the gap, as \( H \) for the commensurate approximant can be written first Chern numbers.

\[ \theta \]

TABLE I. Twist angle \( \theta \) and the indeces \((p_1, p_2, p_3, p_4; q_1, q_2, q_3, q_4) \) of the commensurate approximants (a) to (f). The \( r[Q_{m,n}] \) is the number of the occupied bands below the gap \( Q_{m,n} \).

| (a)  | 29.4093 | 3 8 8 3 | –8 11 | –3 11 | 24 | 28 | 76 | 90 | 142 | 270 |
|------|---------|--------|------|------|----|----|----|----|-----|-----|
| (b)  | 29.5046 | 3 8 8 3 | –9 34 | 9 25 | 43 | 50 | 136 | 161 | 254 | 483 |
| (c)  | 29.6566 | 25 9 34 | –9 27 | 37 | –10 | 37 | 290 | 336 | 916 | 1084 | 1710 | 3252 |
| (d)  | 29.8417 | 11 4 15 | –4 4 15 | 4 11 | 45 | 52 | 142 | 168 | 265 | 504 |
| (e)  | 29.9576 | 11 30 30 | 11 | –30 | 41 | –11 | 41 | 336 | 388 | 1060 | 1254 | 1978 | 3762 |
| (f)  | 30.0579 | 11 30 30 | 11 | –11 | 15 | –4 15 | 123 | 142 | 388 | 459 | 724 | 1377 |

where

\[ C_{i1} = \sum_{j \neq i} \nu_{ij} q_j, \quad C_{i2} = -\sum_{j \neq i} \nu_{ij} p_j \quad (A10) \]

are the integers to characterize the pumping in units of the commensurate period. By using Eqs. (A10) and (A7), we have the Diophantine equation for \( C_{il}'s \),

\[ \sum_{i=1}^{4} p_i C_{i1} = r, \quad \sum_{i=1}^{4} p_i C_{i2} = 0, \]

\[ \sum_{i=1}^{4} q_i C_{i1} = 0, \quad \sum_{i=1}^{4} q_i C_{i2} = -r, \quad (A11) \]

which agrees with the results in the previous work. The Bloch Hamiltonian for the commensurate approximant can be written as \( H(k_1, k_2; \phi_1, \phi_2, \phi_3, \phi_4) \) where \( k_l = k \cdot a_l^i/|a_l^i| (l = 1, 2) \) is the component of the Bloch wavevector along \( a_l^i \), and \( \phi_i (i = 1, 2, 3, 4) \) is the phase factors for the potential slide [Eq. (21)]. Then \( C_{il} \) is given by the first Chern number on a 2D torus of \((k_1, \phi_1)\), or

\[ C_{il} = \frac{1}{2\pi} \int_0^{2\pi} dk_1 \int_0^{2\pi} d\phi_1 F_{il} \in \mathbb{Z}, \quad (A12) \]

where \( F_{il} \) is the Berry curvature defined by

\[ F_{il} = \partial_{\phi_1} a^{(2)} - \partial_2 a^{(1)}, \]

\[ a^{(\mu)} = -i \sum_{\mathbf{k} \in \text{occ}} \langle \alpha, \mathbf{k} | \partial_{\mu} | \alpha, \mathbf{k} \rangle, \quad (A13) \]

and \( \partial_1 = \partial/\partial k_1 \) and \( \partial_2 = \partial/\partial \phi_1 \). The integral period of \( k \) \((0 \leq k \leq |b_l^i|)\) in Eq. (A12) represents the span of the first Brillouin zone in \( l \) direction.

Unlike the second Chern number \( \nu_{ij} \), the first Chern number \( \nu_{ij} \) depends on \( p_i \) and \( q_i \), and hence the systems in Fig. 4 have all different \( C_{il}'s \) for the
calculated for the twisted square potential. The zone 
fold rotational symmetry. The potential amplitude
The potential profile is presented in Fig. 8, for (a)
contrast, the second Chern number \( \nu \) to the span of the corresponding unit cell side. In
M and \( M \) (proportional to the number of bands) is multiplied
reduced to 0 \( i \leq \lvert b_1 \rvert / M \) and, the integrand \( F_{ij} \)
the band folding, the integral path in Eq. (A12) is
M system with a redundant unit cell spanned by
unit cell size can be understood by considering the same
same gap. The direct dependence of \( C_{ij} \) on the unit
cell size can be understood by considering the same
system with a redundant unit cell spanned by \( M_1 \) and \( M_2 \). Due
to the band folding, the integral path in Eq. (A12) is
reduced to 0 \( \leq k_i \leq \lvert b_i \rvert / M \) and, the integrand \( F_{ij} \)
(proportional to the number of bands) is multiplied
\( M_1 M_2 \). As a consequence, the first Chern number
1 \((\nu)\) is given in Sec. III B, which does not depend on the
\( \nu_{ij} \) to the band folding, the integral path in Eq. (A12) is
\( i \leq \lvert b_i \rvert / M \) and, the integrand \( F_{ij} \)
reduced to 0 \( \leq k_i \leq \lvert b_i \rvert / M \) and, the integrand \( F_{ij} \)
(proportional to the number of bands) is multiplied
\( M_1 M_2 \). As a consequence, the first Chern number
\( \nu_{ij} \) to the band folding, the integral path in Eq. (A12) is
reduced to 0 \( \leq k_i \leq \lvert b_i \rvert / M \) and, the integrand \( F_{ij} \)
(proportional to the number of bands) is multiplied
\( M_1 M_2 \). As a consequence, the first Chern number
\( \nu_{ij} \) to the band folding, the integral path in Eq. (A12) is
reduced to 0 \( \leq k_i \leq \lvert b_i \rvert / M \) and, the integrand \( F_{ij} \)
(proportional to the number of bands) is multiplied
\( M_1 M_2 \). As a consequence, the first Chern number

Appendix B: Twisted square potentials

We calculate the energy spectrum and the zone quantum numbers for a twisted double square potential. The Hamiltonian is given by Eq. (1) with

\[
V^\lambda(r) = 2V_0 \sum_{\mu=1}^{2} \cos[b^\lambda_\mu \cdot (r - r^0_\mu)], \tag{B1}
\]

where

\[
b^\alpha_1 = \frac{2\pi}{a} \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad b^\alpha_2 = \frac{2\pi}{a} \begin{pmatrix} 0 \\ 1 \end{pmatrix},
\]

\[
b^{\beta}_{\mu} = R(\theta) b^{\alpha}_{\mu}. \tag{B2}
\]

The corresponding primitive lattice vectors are

\[
a^{\alpha}_1 = a \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad a^{\alpha}_2 = a \begin{pmatrix} 0 \\ 1 \end{pmatrix},
\]

\[
a^{\beta}_{\mu} = R(\theta) a^{\alpha}_{\mu}. \tag{B3}
\]

The potential profile is presented in Fig. 8 for (a) single potential, (b) double potential with \( \theta = 75^\circ \) and (c) \( \theta = 45^\circ \). The system (c) is a quasicrystal with 8-fold rotational symmetry. The potential amplitude is taken as \( V_0 = 0.213\varepsilon_0 \), where \( \varepsilon_0 = \hbar^2/(2ma^2) \).

Figure 9 is a set of plots similar to Fig. 3 calculated for the twisted square potential. The zone quantum numbers are presented in the bottom of

Appendix C: Charge pumping formula from the infinitesimal potential limit

Here we present an alternative method to derive the relation of the charge pumping to the electron density, Eq. (22), by integrating the Berry curvature in the infinitesimal potential limit. First, let us consider a 1D system with a single periodic potential,

\[
H(\phi) = \frac{p^2}{2m} + V(x - \phi/a), \tag{C1}
\]

where \( V(x) \) is a periodic potential with the period of \( a = 2\pi/b \), and the phase \( \phi \) describes sliding of the potential. If we write the periodic potential in a Fourier series as \( V(x) = \sum_m V_m e^{imbx} \), the translated potential is expressed as

\[
V(x - \phi/a) = \sum_m V_m e^{-im\phi} e^{imbx}. \tag{C2}
\]

The electric polarization can be calculated by

\[
P(\phi) = \sum_{n \in occ.} \int_{-b/2}^{b/2} \frac{dk}{2\pi} i\langle u_{nk}(\phi)|\frac{\partial}{\partial k}|u_{nk}(\phi)\rangle \tag{C3}
\]

where \( u_{nk}(\phi) \) is the Bloch eigen state of the \( n \)-th band in the Hamiltonian at phase shift \( \phi \), and occ. represents the occupied bands below the Fermi energy. The charge transport during a single sliding process is given by \( \Delta P = \int_0^{2\pi} d\phi (\partial P/\partial \phi) \). It is expressed as the Chern number on \( (k, \phi) \) space,

\[
\Delta P = \sum_{n \in occ.} \int_0^{2\pi} d\phi \int_{-b/2}^{b/2} \frac{dk}{2\pi} F_n(k,\phi) \tag{C4}
\]

where \( F_n(k,\phi) \) is the Berry curvature defined by

\[
F_n(k,\phi) = \partial_1 a_n^{(2)} - \partial_2 a_n^{(1)},
\]

\[
a_n^{(i)}(k,\phi) = -i\langle u_{nk}(\phi)|\partial_i|u_{nk}(\phi)\rangle, \tag{C5}
\]

and \( \partial_1 = \partial/\partial k \) and \( \partial_2 = \partial/\partial \phi \).

The \( \Delta P \) can be easily calculated by considering an infinitesimal potential limit \( V(x) \to 0 \). When \( V \) is
slightly increased from zero, energy gaps open at \( k = \pm mb/2 \) \( (m = 1, 2, 3, \cdots) \) in the original parabolic band of free electron as illustrated in Fig. 11. Let us consider the eigenstates of the first band, \( u_{1,k} \) in the first Brillouin zone \(-b/2 \leq k \leq b/2\). It is written as \( |u_{1,k}\rangle = \sum_m c_m e^{i(k+mb)x} \) and we fix the global phase such that \( c_0 \) is real. At the edges of the Brillouin zone, we have

\[
|u_{1,b/2}(\phi)\rangle \approx \frac{1}{\sqrt{2}} e^{i(b/2)x} + e^{i\phi} e^{i(-b/2)x} \\
|u_{1,-b/2}(\phi)\rangle \approx \frac{e^{-i\phi}}{\sqrt{2}} e^{i(b/2)x} + \frac{1}{\sqrt{2}} e^{i(-b/2)x}.
\]

They are the same states but differ in the global phase factor by \( e^{i\phi} \). By using the Stokes theorem to

FIG. 8. Contour plots of (a) single square potential, and (b) twisted double square potential with \( \theta = 7^\circ \) and (c) \( \theta = 45^\circ \) [Eq. (B1)].

FIG. 9. Similar plots to Fig. 3 calculated for the twisted double square potential.
$\Delta P = \frac{1}{2\pi} \int_{0}^{2\pi} d\phi [a_{1}^{(2)}(b/2, \phi) - a_{1}^{(2)}(-b/2, \phi)]$ (C7)

Since $|u_{1,b/2}(\phi)\rangle = e^{i\phi}|u_{1,-b/2}(\phi)\rangle$, we find $a_{1}^{(2)}(b/2, \phi) = a_{1}^{(2)}(-b/2, \phi) + 2\pi$, and $\Delta P = 1$ is concluded. In increasing the potential $V$, the Chern numbers do not change as long as the gap remains opening.

The charge pumping for $m$-th gap at $k = \pm mb/2$ can also be calculated in the same manner. We note that any perturbational processes to open the $m$-th gap share the same $\phi$-dependent phase factor $e^{-im\phi}$. For instance, the first order process of $m$-th harmonics has an amplitude of $V_{m}e^{-im\phi}$ and the $m$-th order process of the first harmonics is proportional to $(V_{e}e^{-i\bar{\phi}})^{m}$. We can integrate the Berry curvature for the 2D torus of $-mb/2 \leq k \leq mb/2$ and $0 \leq \phi \leq 2\pi$ just as for the first gap. Noting that the phase factor $e^{-i\phi}$ for the first gap is just replaced with $e^{-im\phi}$, we conclude $\Delta P = m$. Here we neglected all the gaps in the occupied states below $m$-th gap, because they do not affect the sum of the Berry curvature.

The argument also applies to a 1D doubly-periodic system of Eq. (15). When the potential is increased from zero, energy gaps open at $k = \pm mb/2$ and $0 \leq \phi \leq 2\pi$. The corresponding matrix element has the phase factor $e^{-i(m_{1}\phi_{1} + m_{2}\phi_{2})}$. The charge pumping under a unit slide of the potential $V_{i}$ is calculated by integrating the Berry curvature on $(k, \phi_{i})$ space, to obtain $\Delta P_{i} = m_{i}$. It agrees with the results in Sec. IIIA.

The argument can be extended in a straightforward manner to a 2D doubly-periodic system, Eq. (15). We consider a potential sliding expressed by Eq. (19), and calculate the change of the polarization.
The polarization change along the discussion for the 1D case, the corresponding polarization vector. For illustration, we take symmetric pair connected by the reciprocal lattice vector. We can relate the polarization change Eq. (C8) to the derivative of the electronic density as follows. The electronic density $n_e$ for below the gap is given by the area of the qBZ divided by $(2\pi)^2$. When $b_i$ is changed by $\delta b_i$, $G_n$ changes by $\delta G_n = m_{ni}\delta b_i$, and it contributes to the change of the qBZ area by $|q_n|\delta G_n = q_n(G_n \cdot (m_{ni}\delta b_i))/|G_n|$. As a result, the change of the electron density becomes

$$\delta n_e = \frac{1}{2\pi} \frac{1}{(2\pi)^2} \frac{|q_n|}{|G_n|} \cdot \frac{G \cdot (m_{ni}\delta b_i)}{|G_n|},$$

where we used Eq. (C8). This immediately gives

$$\frac{\partial n_e}{\partial b_i} = \frac{1}{2\pi} \Delta P_i,$$

which is Eq. (22).

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