

Gap labeling theorem for multilayer thin film heterostructures

Mao Yoshii¹,* Sota Kitamura¹, and Takahiro Morimoto¹

Department of Applied Physics, The University of Tokyo, Hongo, Tokyo 113-8656, Japan



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Quasiperiodic systems show a universal gap structure due to quasiperiodicity, which is analogous to gap openings at the Brillouin zone boundary in periodic systems. The integrated density of states (IDoS) below those energy gaps is characterized by a few integers, which is known as the “gap labeling theorem” (GLT) for quasiperiodic systems. In this study, focusing on multilayer thin film systems such as twisted bilayer graphene and stacked transition-metal dichalcogenides, we extend the GLT for multilayer systems of arbitrary dimensions and number of layers, using an approach based on the algebra called “a noncommutative torus.” We find that the energy gaps and the associated IDoS are generally characterized by $_{DN}C_D$ integer labels in N layer systems in the D dimensions, when the effect of the interlayer coupling can be approximated by a quasiperiodic intralayer coupling for each layer. We demonstrate that the generalized GLT holds for quasiperiodic 1D tight-binding models by numerical simulations.

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I. INTRODUCTION

Quasiperiodic systems are systems that possess long-range order without translational symmetry. In 1982, quasiperiodic structure was discovered in a system of alloys [1], and quasiperiodicity was later found in various systems [2–6]. The structure of quasiperiodic crystals can be regarded as a projection of higher-dimensional crystalline structure [7,8], and it would allow us to access the physics of higher-dimensional space that is usually inaccessible in three-dimensional crystals. Recently, a stacked system of two-dimensional thin films was realized and studied intensively, including twisted bilayer graphenes [9–11] and the interface of transition-metal dichalcogenides [12,13]. Multilayer systems made up of different crystals can also be considered quasiperiodic systems [13,14]. They provide an interesting platform for quasiperiodic structures due to their controllability and a rich variety of material combinations.

In periodic systems, the energy gap often opens at the Brillouin zone (BZ) boundary due to anticrossing of energy bands that are related by the reciprocal vectors. Similarly, in quasiperiodic systems there exist energy gaps that originate from quasiperiodicity. In quasiperiodic systems, BZ folding takes place in the momentum space picture, and it leads to replicas of energy bands that exhibit anticrossings. Since those energy gaps stem from the geometry of quasiperiodic systems, one can relate the energy gaps with the geometric parameters of the system. Since the energy structure of quasiperiodic systems cannot be captured by the energy dispersion in the momentum space picture in general, understanding the energy gap structure independent of the system size is particularly important. For example, it is known that gaps in the energy spectrum of Fibonacci quasicrystal can be labeled by two integers [15–18]. Using those gap labels, one can discuss the

physical property of the energy gaps regardless of the system size.

Multilayer thin films (MLTFs) show a universal energy gap structure that comes from the quasiperiodicity. Such a gap structure can be understood using the so-called “gap labeling theorem” (GLT). The GLT establishes a relationship between those energy gaps with the integrated density of states (IDoS) below the gap through integer labels, and it has been known for quasicrystals for several decades [17,18]. A GLT for MLTFs was originally proposed using an algebra called a noncommutative torus (NCT) in the case of two-dimensional homobilayer systems (which are made of the same type of atomic layers) [19]. In Ref. [19], the GLT for a twisted bilayer system consisting of the same type of atomic layers was derived, which states that the IDoS below a certain energy gap G is given by

$$\text{IDoS}(G) = n_0 + \sum_{i,j=1,2} n_{ij} \frac{|\mathbf{a}_i \times \mathbf{b}_j|}{S}, \quad (n_{ij} \in \mathbb{Z}). \quad (1)$$

Here, \mathbf{a}_i is a primitive vector of one layer, \mathbf{b}_j is a primitive vector of the other layer, and S is $|\mathbf{a}_1 \times \mathbf{a}_2|$. Namely, the GLT gives a labeling for the IDoS below the energy gap G with integers n .

The GLT is also useful to understand the behavior of the energy gaps when one changes a parameter that characterizes the quasiperiodic system. For example, if we consider a twisted bilayer system, $|\mathbf{a}_i \times \mathbf{b}_j|$ changes continuously with varying the twist angle [Fig. 1(a)]. In this case, the energy gaps for two twist angles can be smoothly connected with each other when the corresponding IDoS has the same label n , as depicted by the dashed curve in Fig. 1(b). More recently, it has been pointed out that such an energy gap structure can also be understood from charge transport that appears when sliding two thin films relatively, which is characterized by a topological quantity called the sliding Chern number (SCN) [20,21].

*mao@g.ecc.u-tokyo.ac.jp

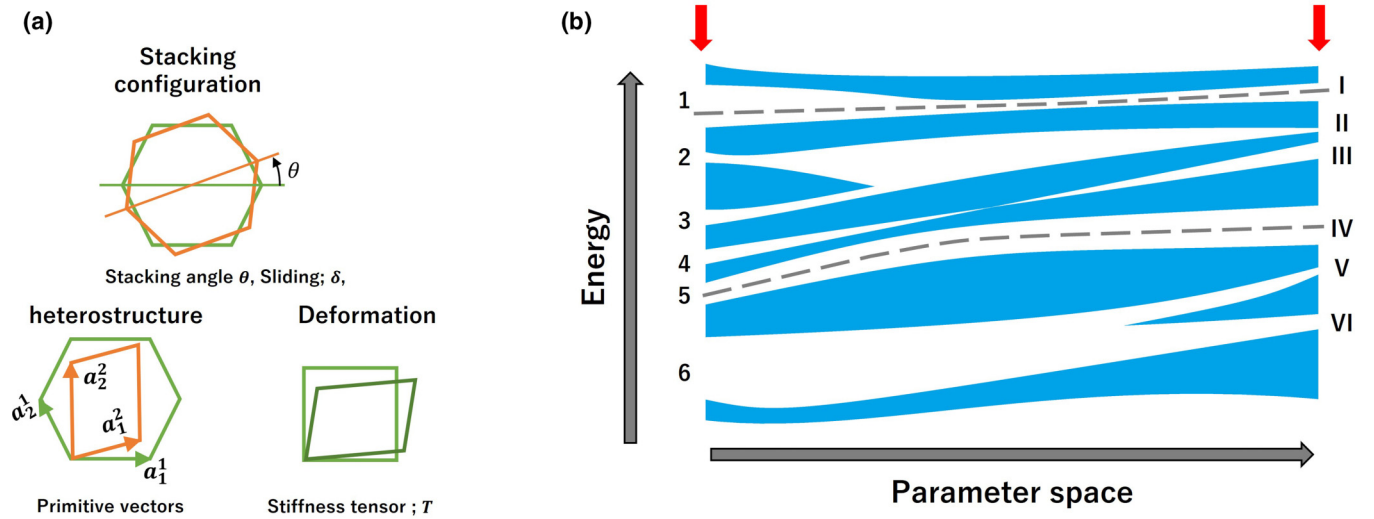


FIG. 1. (a) Parameters that characterize the MLTFs. They include stacking angle, lattice constants of the stacked layers, and deformation strength. (b) A schematic picture of the energy spectrum of MLTFs when one changes the parameters characterizing the MLTFs. Blue regions represent the energy bands, and white regions represent the energy gaps. Gray dashed lines are the energy gaps that originate from the quasiperiodicity and can be captured by the GLT. Those energy gaps show a robust behavior, while other nonuniversal gaps originating from band hybridizations can merge or split when the parameters are changed.

Since derivation of the GLT from the NCT approach only requires information on the quasiperiodic lattice structure, the NCT approach is concise and systematic compared to the SCN approach. So far, the NCT approach for the GLT has only been applied for two-dimensional homobilayer systems [19]. Hence, it is an interesting problem to extend the NCT method to MLTF heterostructures made of different types of two-dimensional (2D) systems. An obstacle in extending the NCT approach for MLTF heterostructures is that the information on the relative size of the unit cells of different layers is not incorporated in the original NCT construction, while it is indispensable to derive GLT for multilayer thin films. Also, previous studies on homobilayer systems [19–21] derived GLT by focusing on the IDoS of one layer, since the system is invariant under exchanging the two layers in homobilayer systems, which is no longer the case for general MLTF heterostructures. Therefore, to understand the electronic structure of general MLTFs, it is necessary to treat the electronic structure of all layers on an equal footing.

In this paper, we extend the NCT approach for the GLT to MLTF heterostructures. To this end, we adopt an approach from the approximately finite C^* -algebra [22,23]. Specifically, we relate the traces for the different layers using the inductive limit for the parameters characterizing the NCT obtained from the continued fraction, which is effectively equivalent to considering large approximants of MLTF heterostructures. Assuming that the interlayer coupling is approximated by quasiperiodic intralayer couplings for each layer, which generally holds when states in different layers are energetically separated, we extend the GLT for MLTF heterostructures. The generalized GLT reveals that the IDoS for N -layer heterostructures in D dimensions is characterized by $_{DN}C_D$ integer labels. We perform numerical simulations for tight-binding models of 1D MLTF heterostructures, and we demonstrate that the generalized GLT indeed holds.

The rest of the paper is organized as follows. In Sec. II, we review the GLT for MLTFs consisting of the same type of atomic layers, and we introduce algebraic structure of operators in the MLTFs. In Sec. III, we first extend the GLT to the bilayer heterostructures in one dimension and then to the general N -layer systems in arbitrary dimensions in Sec. IV. In Sec. V, we show numerical calculation in a one-dimensional MLTF heterostructure system to demonstrate that the generalized GLT holds.

II. GAP LABELING THEOREM

In this section, we briefly introduce the original gap labeling theorem [16–18]. In periodic systems, band folding at the Brillouin zone boundary often leads to anticrossing between folded bands and gap opening. When the energy gap appears from such band folding, the IDoS below such a gap is given by an integer times the BZ volume. In quasiperiodic systems, a gap opening also appears from the band folding due to the quasiperiodic structure, and a similar relationship for IDoS holds, which is known as GLT.

To explain the GLT, we first define the IDoS as follows. Let \hat{H} be a Hamiltonian with energy eigenvalues $E_1 \leq \dots \leq E_{\dim \hat{H}}$ and eigenstates $\{|\psi_n\rangle\}$, ($n \in \{1, \dots, \dim \hat{H}\}$). We denote the projector to the states below the energy E as

$$\hat{P}(E) = \sum_{E_i \leq E} |\psi_i\rangle\langle\psi_i|. \quad (2)$$

Since we mainly concentrate on energy gaps in this paper, it is convenient to relate $\hat{P}(E)$ to energy gaps. When we refer to the energy gap between E_n and E_{n+1} as G , we also write $\hat{P}(G) := \hat{P}(E_n)$. Using the projector, IDoS is defined as

$$\text{IDoS}(E) = \tau(\hat{P}(E)), \quad (3)$$

$$\tau(\hat{O}) = \frac{1}{\dim(\hat{O})} \text{Tr}(\hat{O}). \quad (4)$$

Here, τ is the normalized trace defined so that τ of identity operator $\mathbf{1}$ becomes 1. In the same manner, we also write it as IDoS(G) = $\tau(\hat{P}(G))$. While we can define the normalized trace as in Eq. (3) for finite dimensions, in the case of infinite dimensions we adopt the inductive limit from finite-dimensional matrix algebras for construction of NCT and a definition of τ [with Eq. (3)] [24–26]. In the rest of this section, to explain the GLT, we explicitly derive the GLT for a toy model.

A. Gap labeling theorem in one dimension

To extend the formalism of Ref. [19], let us review the original GLT in the case of one dimension using the so-called Harper model.

First, we demonstrate that the Hamiltonian of a lattice under an incommensurate potential can be regarded as an operator on an NC torus. Let us consider the following model:

$$\hat{H} = \sum_n [(t|n+1\rangle\langle n| + \text{H.c.}) + V(n)|n\rangle\langle n|], \quad (5)$$

where $V(x) = V(x + \theta^{-1})$ is a periodic function, which is incommensurate when θ is taken to be irrational. We can expand V into a Fourier series as

$$V(x) = \sum_{\eta \in \mathbb{Z}} v_\eta e^{2\pi i \eta x \theta}. \quad (6)$$

Let us define \hat{S} and \hat{U} as

$$\hat{S} = \sum_n |n-1\rangle\langle n|, \quad (7)$$

$$\hat{U} = \sum_n e^{2\pi i n \theta} |n\rangle\langle n|, \quad (8)$$

which follow the commutation relation

$$\hat{S}\hat{U} = e^{2\pi i \theta} \hat{U}\hat{S}. \quad (9)$$

With these operators, we can write the Hamiltonian as a polynomial of \hat{U} and \hat{S} as

$$\hat{H} = t(\hat{S} + \hat{S}^\dagger) + \sum_{\eta \in \mathbb{Z}} v_\eta \hat{U}^\eta. \quad (10)$$

B. Noncommutative torus

The above commutation relation defines an algebra called a noncommutative torus. The noncommutative D -torus is an algebra of operators $\{\hat{U}_j\}_{j=1,\dots,D}$, which follows the commutation relation

$$\hat{U}_i \hat{U}_j = e^{2\pi i \theta_{ij}} \hat{U}_j \hat{U}_i. \quad (11)$$

Here, θ_{ij} is a real number that characterizes the noncommutative torus, which can be regarded as an element of the antisymmetric matrix θ . We call θ a noncommutative parameter, and we denote a noncommutative D -torus defined by θ as \mathbb{T}_θ^D . For example, a noncommutative two-torus appears in the context of Hofstadter's butterfly in quantum Hall systems. In a noncommutative D -torus, we can also construct a projection operator, whose trace is directly related to the IDoS. For any Hamiltonian in an algebra of the noncommutative D -torus

\mathbb{T}_θ^D , it is known that the IDoS of the state below energy gap G is expressed using θ as [27]

$$\text{IDoS}(G) = n_\emptyset + \sum_{J \subset \{1,\dots,D\}} n_J \text{Pf}(\theta_J), \quad (12)$$

where the subscript J labels subsets of $\{1, \dots, D\}$, Pf denotes a Pfaffian, and θ_J is a submatrix of θ defined as

$$\{\theta_J\}_{ij} = \begin{cases} \theta_{ij}, & (i, j \in J), \\ 0, & \text{others.} \end{cases} \quad (13)$$

Once we obtain the parameter θ for the quasiperiodic system, application of the above formulas leads to the expression for the IDoS.

For the case of Eq. (5), \hat{H} is an operator belonging to the NCT of parameter θ , and the associated IDoS is given by

$$\text{IDoS}(G) = n_\emptyset + \theta n_1. \quad (14)$$

III. GAP LABELING THEOREM OF ONE-DIMENSIONAL MULTILAYER THIN FILMS

In this section we focus on a one-dimensional system, and we derive the generalized GLT for MLTF heterostructures using the NCT approach, which is consistent with those obtained from other approaches [20,28].

One obstacle in extending the GLT is the relation of the normalized trace τ in MLTF systems. As we show below, we compute the gap labels of the MLTF heterostructures by approximately decoupling layers and applying the NCT approach to each layer. However, since the normalized trace τ has a different normalization factor for a different Hilbert space, the IDoS of the entire MLTF is not simply obtained as a sum of the IDoS of each layer. To derive the gap label for the MLTFs, we need to know the relation between the τ 's defined in each layer. Specifically, for the infinite-dimensional case, we take an inductive limit with finite-dimensional matrix algebras, where the relation of the normalized trace for different layers is incorporated in a straightforward way. This approach is known as approximately finite (AF) algebra [22–24].

In this section we focus on one-dimensional MLTF heterostructures, and we apply the above operations to derive the generalized GLT. We mostly consider the bilayer case, and we mention the general N -layer systems in the end.

A. Hamiltonian for a quasiperiodic bilayer

We construct a Hamiltonian \hat{H} for a quasiperiodic bilayer by coupling two single-layer tight-binding models (we denote the single-layer model of layer l as \hat{H}^l) with interlayer coupling \hat{W} ,

$$\hat{H} = \hat{H}^1 + \hat{H}^2 + \hat{W} + \hat{W}^\dagger. \quad (15)$$

Here, the single-layer Hamiltonian \hat{H}^l does not depend on the other layers, and it has no internal degrees of freedom (such as sublattice degrees of freedom) for simplicity. Namely,

$$\hat{H}^l = \sum_{n', m' \in \mathbb{Z}} h_{n' - m'} |n', l\rangle\langle m', l|. \quad (16)$$

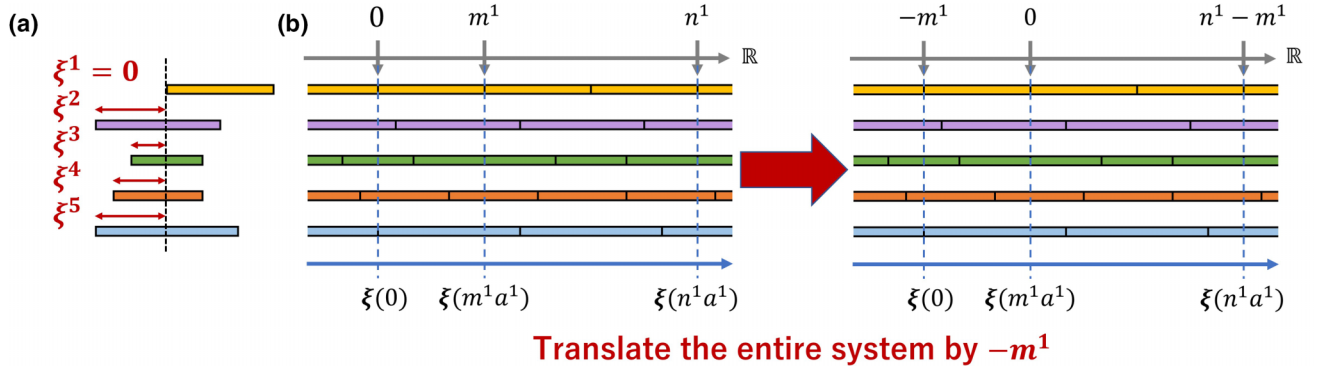


FIG. 2. A schematic picture of the parameter ξ characterizing the layer stacking of the MLTFs. (a) Example of $\xi(r)$ of an electron on layer 1. We focus on a particular unit cell in layer 1, and we suppose that the electron is located at the position ξ^1 . ($\xi^1 = 0$ corresponds to the base point of the unit cell in layer 1.) For the layer l other than 1, we define parameter ξ^l by a position of the same electron measured within the unit cell of layer l . In the tight-binding model, electrons are bound to the lattice sites, and $\xi^1 = 0$. (b) Translation of the layers and ξ . When we translate the layers by $-m^1 a^1$, the original parameter $\xi(0)$ is replaced by $\xi(m^1 a^1)$.

Here, n^l and m^l are the labels of sites on layer l . Hereafter, we omit the second (layer) index l for states as it is apparent from the superscript of the first (site) index n^l . The position of site n^l is defined as $n^l a^l$, with a^l being the lattice constant of layer l . From the periodicity of layer l , the hopping amplitude h depends only on the relative distance between site n^l and site m^l . In contrast, the interlayer coupling \hat{W} depends on how the two layers are stacked. We express \hat{W} by a fully connected model as

$$\hat{W} = \sum_{n^1, m^2} W(n^1, m^2) |n^1\rangle \langle m^2|. \quad (17)$$

B. Effective Hamiltonian in each layer

The GLT from the NCT approach can capture a gap structure that arises from the quasiperiodicity, which we call the intraband energy gap. Such an energy gap originates from a gap opening for folded bands due to a lattice constant mismatch, and it appears at the Bragg lines, which is analogous to the gap opening at the BZ boundary in periodic systems. On the other hand, interlayer coupling in MLTFs also causes hybridization between different bands, and it leads to a gap opening that is not directly related to the quasiperiodic nature, which we call the interband energy gap. To capture the universal gap structure of intraband energy gaps by the NCT approach, below we approximate the interlayer couplings in Eq. (15) with quasiperiodic intralayer couplings. This approximation is justified as far as energy bands of different layers are energetically separated and the interlayer coupling is not too large.

When we define a projector onto the space in layer l as \hat{P}^l , we can write the equation $\hat{H}|\psi\rangle = E|\psi\rangle$ as

$$E\hat{P}^1|\psi\rangle = \hat{H}^1\hat{P}^1|\psi\rangle + \hat{W}\hat{P}^2|\psi\rangle, \quad (18)$$

$$E\hat{P}^2|\psi\rangle = \hat{W}^\dagger\hat{P}^1|\psi\rangle + \hat{H}^2\hat{P}^2|\psi\rangle, \quad (19)$$

and the effective Hamiltonian in layer l is

$$\hat{H}_{\text{eff}}^1(E) = \hat{H}^1 + \hat{W} \frac{1}{E - \hat{H}^2} \hat{W}^\dagger, \quad (20)$$

$$\hat{H}_{\text{eff}}^2(E) = \hat{H}^2 + \hat{W}^\dagger \frac{1}{E - \hat{H}^1} \hat{W}. \quad (21)$$

In the following, we approximate E of $H_{\text{eff}}^1(H_{\text{eff}}^2)$ with some constant which is comparable with eigenvalues of $H^1(H^2)$ of interest. The second term of each line is the quasiperiodic term that behaves as an intraband coupling subject to the quasiperiodic pattern. We denote such quasiperiodic intralayer coupling in layer l as \hat{V}^l , which can be formally expressed as

$$\hat{V}^l = \sum_{n^l, m^l} \tilde{V}^l(n^l, m^l, \xi(0)) |n^l\rangle \langle m^l|. \quad (22)$$

Here, ξ^l is a function of $r \in \mathbb{R}$, which specifies the position in the unit cell of layer l [19]. As depicted in Fig. 2(a), an electron at one layer defines the positions in unit cells of other layers ξ^l . For a general position r for an electron, collecting the position $\xi^l(r)$ in the unit cell of each layer, we write $\xi(r) = \{\xi^1(r), \dots, \xi^N(r)\}$, which determines the stacking configuration of the unit cells of different layers at the position r . From the periodicity of layers, specifying how we stack unit cells is equivalent to specifying how we stack layers. Thus, ξ at some point r specifies the quasiperiodic pattern of the MLTF heterostructure. We mainly use $\xi(0)$ to specify the quasiperiodic pattern in the following sections.

Next, we consider a term $\tilde{V}^l(n^l, m^l, \xi(0))$. This represents the hopping process where an electron at site m^l hops to n^l in the MLTFs specified by $\xi(0)$. When we translate the system by $-m^l a^l$, site n^l is translated to $n^l - m^l$, and site m^l is at site 0. Regarding ξ , the $\xi(0)$ of the translated system corresponds to $\xi(m^l a^l)$ in the original system [Fig. 2(b)]. Hence, $\tilde{V}^l(n^l, m^l, \xi(0))$ coincides with $\tilde{V}^l(n^l - m^l, 0, \xi(m^l a^l))$ after the translation. Therefore, omitting 0 in the second argument, we can write \hat{V}^l as

$$\hat{V}^l = \sum_{n^l, m^l} \tilde{V}^l(n^l - m^l, \xi(m^l a^l)) |n^l\rangle \langle m^l|. \quad (23)$$

When we consider layer l under the tight-binding approximation, electrons are bound to the sites with no internal degrees of freedom. In this case, $\xi^l(m^l a^l) = 0$, and we may omit ξ^l from ξ .

C. Fourier expansion

Next, we expand \hat{V}^l in a Fourier series. First, we consider the layer $l = 1$ and define $q^1 = n^1 - m^1$. Applying the discussions in Sec. III B to a bilayer system, ξ^2 has the periodicity $\xi^2(m^1 a^1 + a^2) = \xi^2(m^1 a^1)$. Using this periodicity, we expand the quasiperiodic intralayer coupling in the Fourier series as

$$V^1(q^1, \xi^2(m^1 a^1)) = \sum_{\eta^1 \in \mathbb{Z}} v_{q^1, \eta^1} e^{2\pi i \eta^1 \frac{\xi^2(m^1 a^1)}{a^2}}. \quad (24)$$

Defining the slide operator as $\hat{S}^1 = \sum_n |n^1 - 1\rangle \langle n^1|$, we can write

$$\hat{V}^1 = \sum_{m^1, q^1} \sum_{\eta^1} v_{q^1, \eta^1} e^{2\pi i \eta^1 \frac{m^1 a^1}{a^2}} (\hat{S}^{1\dagger})^{q^1} |m^1\rangle \langle m^1| + \text{H.c.}, \quad (25)$$

where we have used $e^{2\pi i \frac{\xi^2(m^1 a^1)}{a^2}} = e^{2\pi i \frac{m^1 a^1}{a^2}}$. Defining the generator \hat{U}_1 as $\sum_{m^1} e^{2\pi i \frac{m^1 a^1}{a^2}} |m^1\rangle \langle m^1|$, we rewrite the above equation as

$$\hat{V}^1 = \sum_{q^1} \sum_{\eta^1} v_{q^1, \eta^1} (\hat{S}^{1\dagger})^{q^1} \hat{U}_1^{\eta^1} + \text{H.c.} \quad (26)$$

In this manner, we can express quasiperiodic intralayer coupling as a polynomial of \hat{U}_1 and \hat{S}^1 . In the same procedure, we can also decompose quasiperiodic intralayer coupling in layer 2 as

$$\hat{V}^2 = \sum_{q^2} \sum_{\eta^2} v_{q^2, \eta^2} (\hat{S}^{2\dagger})^{q^2} \hat{U}_2^{\eta^2} + \text{H.c.}, \quad (27)$$

$$\hat{U}_2 = \sum_{m^2} e^{2\pi i \frac{m^2 a^2}{a^1}} |m^2\rangle \langle m^2|, \quad (28)$$

$$\hat{S}^2 = \sum_{m^2} |m^2 - 1\rangle \langle m^2|. \quad (29)$$

D. Noncommutativity between translation and generator

To define a noncommutative torus, we define \hat{U}_3 and \hat{U}_4 by

$$\hat{U}_3 = \hat{S}^1, \quad (30)$$

$$\hat{U}_4 = \hat{S}^2. \quad (31)$$

Then, \hat{U}_i 's satisfy the following commutation relations:

$$\hat{U}_1 \hat{U}_3 = e^{-2\pi i \frac{a^1}{a^2}} \hat{U}_3 \hat{U}_1, \quad (32)$$

$$\hat{U}_2 \hat{U}_4 = e^{-2\pi i \frac{a^2}{a^1}} \hat{U}_4 \hat{U}_2. \quad (33)$$

From these relations, we construct a noncommutative torus generated by (\hat{U}_1, \hat{U}_3) and (\hat{U}_2, \hat{U}_4) . The parameter θ of the corresponding NCT is obtained from the commutation relation $\hat{U}_i \hat{U}_j = e^{-2\pi i \theta_{ij}} \hat{U}_j \hat{U}_i$ as

$$\theta_{13} = \frac{a^1}{a^2}, \quad (34)$$

$$\theta_{24} = \frac{a^2}{a^1}. \quad (35)$$

Hence, the effective Hamiltonian on each layer can be expressed as an operator defined on the noncommutative torus $\mathbb{T}_{\theta_{13}}$ and $\mathbb{T}_{\theta_{24}}$, and the total (effective) Hamiltonian of the

bilayer system becomes an element of the algebra $\mathbb{T}_{\theta_{13}} \oplus \mathbb{T}_{\theta_{24}}$. Thus the projector of the bilayer Hamiltonian is expressed as

$$\hat{P} = \hat{P}^1 \oplus \hat{P}^2, \quad (36)$$

where \hat{P} is the projector in $\mathbb{T}_{\theta_{13}} \oplus \mathbb{T}_{\theta_{24}}$, and \hat{P}^l is the projector in the layer l . Here, it is worth noting that the relation between the normalized trace of the bilayer system is not simply given by a summation of the normalized trace of layer l as $\tau(\hat{P}) = \tau^1(\hat{P}^1) + \tau^2(\hat{P}^2)$, because the normalized trace τ^l is defined in a different subspace for each layer. Therefore, to derive the GLT, we should examine the relation between τ^1 and τ^2 . Directly relating τ^1 and τ^2 is hard since the dimension of \hat{U}_i is infinity, as we have defined in Sec. III C. To overcome this issue, we use the AF algebra [26,29]. This algebra defines the NCT as the inductive limit of the finite-dimensional matrix algebra, where we can relate the normalized traces for different layers more easily.

In the following, we follow the approach by Primisner and Voiculescu [23] to relate the traces in different layers. First, one represents θ with a continued fraction,

$$\theta = z_0 + \frac{1}{z_1 + \frac{1}{z_2 + \frac{1}{z_3 + \dots}}} = [z_0; z_1, \dots], \quad (37)$$

and then one approximates θ with an approximant of θ defined as

$$\theta_n = z_0 + \frac{1}{\dots + \frac{1}{z_n}} = \frac{p_n}{q_n}, \quad (38)$$

where p_n and q_n are coprime integers. When we approximate θ by θ_n , we can represent the generators of the noncommutative torus with q_n -dimensional matrices and define IDoS using a trace of the finite-size matrices. Next, to construct $\mathbb{T}_{\theta_{n+1}}^2$, we embed $\mathbb{T}_{\theta_n}^2$ and $\mathbb{T}_{\theta_{n-1}}^2$ to a q_{n+1} -dimensional matrix with a suitable unitary transformation [for details, see Eq. (2) in Ref. [23]]. Continuing this embedding, we define \mathbb{T}_{θ}^2 as an inductive limit, $\mathbb{T}_{\theta}^2 = \lim_{n \rightarrow \infty} \mathbb{T}_{\theta_n}^2$. In this construction, the IDoS of \mathbb{T}_{θ}^2 is also defined as the inductive limit from the IDoS of \mathbb{T}_{θ_n} , which can be defined in the finite-dimensional matrix algebra. When we consider an approximant θ_n for the quasiperiodicity parameter $\theta = a^1/a^2$ for the bilayer system, we effectively consider a superlattice made of q_n sites in layer 1 and p_n sites in layer 2, which we call “the moiré unit cell.” When we consider the system of length p_n with the periodic boundary condition, we may use a phase matrix P_{θ_n} and a clock matrix C_{θ_n} as a representation of \hat{U}_1 and \hat{U}_3 :

$$\{P_{\theta_n = \frac{p_n}{q_n}}\}_{ij} = \begin{cases} e^{2\pi i \theta_n j}, & i = j, \\ 0, & \text{others}, \end{cases} \quad (39)$$

$$\{C_{\theta_n = \frac{p_n}{q_n}}\}_{ij} = \begin{cases} 1, & j - i = 1, \\ 1, & (i, j) = (q_n, 1), \\ 0, & \text{others} \end{cases} \quad (40)$$

for $1 \leq i, j \leq q_n$. Using these matrices, the representations of \hat{U} 's under this approximation are

$$\hat{U}_1 = P_{\theta_n}, \quad (41)$$

$$\hat{U}_2 = P_{\theta_n^{-1}}, \quad (42)$$

$$\hat{U}_3 = C_{\theta_n}, \quad (43)$$

$$\hat{U}_4 = C_{\theta_n^{-1}}. \quad (44)$$

The dimension of \hat{U}_1 and \hat{U}_3 is q_n , and that of \hat{U}_2 and \hat{U}_4 is p_n . Thus, in the finite-dimensional matrix algebra, the IDoS of layer 1 is expressed as

$$\text{IDoS}^1(G) = \frac{1}{q_n} \text{Tr}(\hat{P}(G)). \quad (45)$$

Since the Hamiltonian of the bilayer system is the direct sum of H_{eff}^1 and H_{eff}^2 , the IDoS of the bilayer system and those of layers 1 and 2 satisfy the following relation:

$$(p_n + q_n) \text{IDoS}(G) = q_n \text{IDoS}^1(G) + p_n \text{IDoS}^2(G). \quad (46)$$

According to Ref. [30], the IDoS for each layer is given by $\text{IDoS}^1(G) = n_1^1 + \theta_n n_2^1$ ($n_1^1, n_2^1 \in \mathbb{Z}$) and $\text{IDoS}^2(G) = n_2^2 + \theta_n^{-1} n_1^2$ ($n_1^2, n_2^2 \in \mathbb{Z}$), which leads to

$$\text{IDoS}(G) = (n_1^1 + n_1^2) \frac{q_n}{(p_n + q_n)} + (n_2^1 + n_2^2) \frac{p_n}{(p_n + q_n)}. \quad (47)$$

Taking the inductive limit of $p_n/q_n \rightarrow \theta = a^1/a^2$, we obtain

$$\text{IDoS}(G) = \frac{1}{\frac{1}{a^1} + \frac{1}{a^2}} \left[\frac{n_1}{a^1} + \frac{n_2}{a^2} \right]. \quad (48)$$

Here, $n_k = \sum_{l=1,2} n_k^l$. As a result, we can label IDoS of the bilayer system with two integers. This result is consistent with the previous results including Fig. 6.3 in Ref. [28] and Eq. (A3) in Appendix from the SCN approach.

As one can easily see, q_n is the number of unit cells inside the moiré unit cell of layer 1, and p_n is that of layer 2. Therefore, $q_n/(p_n + q_n)$ is the density of unit cells of layer 1 inside the moiré unit cell. Thus relating the trace of each layer can be intuitively understood as introducing the ratio of the number of unit cells of two layers. This allows us to extend the above formalism to multilayer and higher-dimensional systems in a straightforward way.

In a similar manner, we can also extend GLT to the N -layer system. Considering an N -layer system with lattice constant a^l , we can write IDoS of layer l (IDoS^l) as

$$\text{IDoS}^l = \sum_{l'=1}^N n_{l'}^l \frac{a^l}{a^{l'}}. \quad (49)$$

Here, $\{n_1^l, \dots, n_N^l\}$ are integers. From the relationship between IDoS^l and the IDoS of the entire system,

$$\left(\sum_{l=1}^N \frac{1}{a^l} \right) \text{IDoS} = \sum_l \frac{1}{a^l} \text{IDoS}^l, \quad (50)$$

we obtain

$$\text{IDoS} = \frac{(\sum_{l=1}^N \frac{n_l}{a^l})}{(\sum_{l=1}^N \frac{1}{a^l})} \left(n_{l'} = \sum_l n_{l'}^l \right). \quad (51)$$

IV. GAP LABELING THEOREM OF D -DIMENSIONAL MLTFs

In this section, we extend the GLT to D -dimensional MLTF heterostructures. We first summarize our notations to describe

D -dimensional MLTFs. In D -dimensional MLTFs, we define the i th primitive vector of layer l as \mathbf{a}_i^l , and its reciprocal vector \mathbf{b}_i^l is defined such that $\mathbf{a}_i^l \cdot \mathbf{b}_j^l = \delta_{ij}$. Alternatively, we also denote the i th primitive (reciprocal) vector in layer l as $\mathbf{a}_{(l-1)D+i}^l = \mathbf{a}_i^l$. In a D -dimensional system, we can express the D -dimensional volume of the region spanned by $\mathbf{a}_{i_1}, \dots, \mathbf{a}_{i_D}$ as $S_{i_1 \dots i_D} = |\det(\mathbf{a}_{i_1}, \dots, \mathbf{a}_{i_D})|$. When we replace \mathbf{a}_{i_D} with unit vector \mathbf{e}_D such that $\mathbf{e}_D \cdot \mathbf{a}_{i_j} = 0$ ($j = 1, \dots, D-1$), we can omit the D th index i_D from S and define

$$S_{i_1 \dots i_{D-1}} = |\det(\mathbf{a}_{i_1}, \dots, \mathbf{a}_{i_{D-1}}, \mathbf{e}_D)|. \quad (52)$$

In a similar manner, we can also define $S_{i_1 \dots i_d}$ as

$$S_{i_1 \dots i_d} = |\det(\mathbf{a}_{i_1}, \dots, \mathbf{a}_{i_d}, \mathbf{e}_{d+1}, \dots, \mathbf{e}_D)|, \quad (53)$$

where $\mathbf{a}_i \cdot \mathbf{e}_j = 0$ ($i = i_1, \dots, i_d, j = d+1, \dots, D$). In particular, if some vectors from \mathbf{a}_{i_1} to \mathbf{a}_{i_D} are parallel with each other, $S_{i_1 \dots i_D} = 0$. To label sites in layer l , we use integers $\{n_i^l\}_{i=1, \dots, D}$ and the parameter $\tilde{\mathbf{r}} \in \{\sum_{d=1}^D \tilde{n}_d^l \mathbf{a}_d^l | 0 \leq \tilde{n}_d^l < 1\}$ that specifies the origin of layer l in \mathbb{R}^D space, where the coordinate of the site $\mathbf{r} \in \mathbb{R}^D$ is represented as

$$\mathbf{r} = \sum_{d=1}^D n_d^l \mathbf{a}_d^l + \tilde{\mathbf{r}}. \quad (54)$$

A. 2D systems

First, we extend Ref. [19] to two-dimensional heterobilayer systems. Then, we derive GLT for the two-dimensional multilayer system.

1. Bilayer case

We consider bilayer systems. In this case we have four primitive vectors, and the parameter of the noncommutative torus for layer 1 is given by

$$\theta^1 = \frac{1}{S_{34}} \begin{pmatrix} 0 & 0 & S_{13} & S_{14} \\ 0 & 0 & S_{23} & S_{24} \\ -S_{13} & -S_{23} & 0 & 0 \\ -S_{14} & -S_{24} & 0 & 0 \end{pmatrix}. \quad (55)$$

The derivation of θ^1 is as follows. In layer 1 of the two-dimensional bilayer, the period of the quasiperiodic pattern is equal to the primitive vectors of layer 2. Specifically, omitting $\xi^1(\mathbf{r}) = \mathbf{0}$, we can represent the quasiperiodic coupling term only with $\xi^2(\mathbf{r})$, which is the position of an electron on layer 1 in the unit cell of layer 2. Writing $\xi^2(\mathbf{r}) = \tilde{\xi}_3(\mathbf{r})\mathbf{a}_3 + \tilde{\xi}_4(\mathbf{r})\mathbf{a}_4$ with $\tilde{\xi}_j(\mathbf{r}) \in [0, 1)$, we define

$$\hat{u}_j = \sum_{\mathbf{r}^1 \in \mathbb{R}^2} e^{2\pi i \xi^2(\mathbf{r}^1) \cdot \mathbf{b}_j} |\mathbf{r}^1\rangle \langle \mathbf{r}^1| = \sum_{\mathbf{r}^1 \in \mathbb{R}^2} e^{2\pi i \tilde{\xi}_j(\mathbf{r}^1) \cdot \mathbf{r}^1} |\mathbf{r}^1\rangle \langle \mathbf{r}^1|, \quad (56)$$

where $j = 3, 4$, and \mathbf{r}^1 runs the position of sites in layer 1 in Eq. (54). Denoting the shift operators that translate the layer 1 by $-\mathbf{a}_1$ and $-\mathbf{a}_2$ as \hat{u}_1 and \hat{u}_2 , we obtain

$$\hat{u}_3 \hat{u}_1 = \sum_{\mathbf{r}^1 \in \mathbb{R}^2} e^{2\pi i \xi^2(\mathbf{r}^1 - \mathbf{a}_1) \cdot \mathbf{b}_3} |\mathbf{r}^1 - \mathbf{a}_1\rangle \langle \mathbf{r}^1 - \mathbf{a}_1| \quad (57)$$

and

$$\hat{u}_1 \hat{u}_3 = \sum_{\mathbf{r}^1 \in \mathbb{R}^2} e^{2\pi i \xi^2(\mathbf{r}^1) \cdot \mathbf{b}_3} |\mathbf{r}^1 - \mathbf{a}_1\rangle \langle \mathbf{r}^1 - \mathbf{a}_1|. \quad (58)$$

Hence the commutation relation of \hat{u}_1 and \hat{u}_3 is

$$\hat{u}_1 \hat{u}_3 = e^{2\pi i [\xi^2(r^1) - \xi^2(r^1 - a_1)] \cdot b_3} \hat{u}_3 \hat{u}_1, \quad (59)$$

where this phase factor does not depend on r^1 . Indeed, when we expand a_1 as

$$a_1 = \tilde{\theta}_{13} a_3 + \tilde{\theta}_{14} a_4, \quad (60)$$

$\tilde{\xi}_3(r^1 - a_1) \equiv \tilde{\xi}_3(r^1) - \tilde{\theta}_{13} \pmod{1}$ holds, so that

$$e^{2\pi i [\xi^2(r^1) - \xi^2(r^1 - a_1)] \cdot b_3} = e^{2\pi i \tilde{\theta}_{13}}. \quad (61)$$

From the definition of reciprocal vectors,

$$|\tilde{\theta}_{ij}| = |a_i \cdot b_j| = \frac{S_{i\bar{j}}}{S_{34}}, \quad (62)$$

where $\{j, \bar{j}\} = \{3, 4\}$. As the sign does not affect the derivation of GLT, we may use $S_{i\bar{j}}/S_{34}$ instead of $\tilde{\theta}_{ij}$. Thus, defining

$$(\hat{U}_1, \hat{U}_2, \hat{U}_3, \hat{U}_4) = (\hat{u}_1, \hat{u}_2, \hat{u}_4, \hat{u}_3), \quad (63)$$

we obtain the noncommutative parameters in Eq. (55). Applying Eq. (12) for θ^1 , IDoS of the associated NC torus is given by

$$\begin{aligned} \text{IDoS}^1 &= n_\emptyset^1 + \sum_{J \subset \{1,2,3,4\}} n_J^1 \text{Pf}(\theta_J^1) \\ &= n_\emptyset^1 + \sum_{i=1,2} \sum_{j=3,4} n_{ij}^1 \frac{S_{ij}}{S_{34}} + n_{1234}^1 \frac{S_{12}}{S_{34}}, \end{aligned} \quad (64)$$

where θ_J^1 is a submatrix of θ^1 defined in Eq. (13), and we used the following formula:

$$\begin{aligned} S_{13}S_{24} - S_{23}S_{14} &= (a_1 \times a_3) \cdot (a_2 \times a_4) \\ &\quad - (a_2 \times a_3) \cdot (a_1 \times a_4) \\ &= (a_1 \times a_2) \cdot (a_3 \times a_4) = S_{12}S_{34}. \end{aligned} \quad (65)$$

This result means that we need six integers to label energy gaps of a single layer in a two-dimensional bilayer system, which coincides with the result in Ref. [31].

Similarly, the IDoS for layer 2 is given by

$$\text{IDoS}^2 = n_\emptyset^2 + \sum_{i=1,2} \sum_{j=3,4} n_{ij}^2 \frac{S_{ij}}{S_{12}} + n_{3412}^2 \frac{S_{34}}{S_{12}}. \quad (66)$$

Next, we glue these two tori following the procedure we have discussed in the previous section. As a result, we obtain IDoS of a two-dimensional bilayer system as

$$\text{IDoS} = \frac{1}{S_{12} + S_{34}} \left[\sum_{i=1}^4 \sum_{j=i+1}^4 n_{ij} S_{ij} \right]. \quad (67)$$

2. Trilayer and N -layer cases

First, we consider a two-dimensional trilayer system. In this case, we have six primitive vectors, and the

noncommutative parameter of layer 1 is

$$\theta^1 = \begin{pmatrix} 0 & 0 & \frac{S_{13}}{S_{34}} & \frac{S_{14}}{S_{34}} & \frac{S_{15}}{S_{56}} & \frac{S_{16}}{S_{56}} \\ 0 & 0 & \frac{S_{23}}{S_{34}} & \frac{S_{24}}{S_{34}} & \frac{S_{25}}{S_{56}} & \frac{S_{26}}{S_{56}} \\ -\frac{S_{13}}{S_{34}} & -\frac{S_{23}}{S_{34}} & 0 & 0 & 0 & 0 \\ -\frac{S_{14}}{S_{34}} & -\frac{S_{24}}{S_{34}} & 0 & 0 & 0 & 0 \\ -\frac{S_{15}}{S_{56}} & -\frac{S_{25}}{S_{56}} & 0 & 0 & 0 & 0 \\ -\frac{S_{16}}{S_{56}} & -\frac{S_{26}}{S_{56}} & 0 & 0 & 0 & 0 \end{pmatrix}. \quad (68)$$

From Eq. (12), the IDoS of layer 1 is

$$\begin{aligned} \text{IDoS}^1 &= n_\emptyset^1 + \sum_{i=1,2} \sum_{j=3,4} n_{ij}^1 \frac{S_{ij}}{S_{34}} + \sum_{i=1,2} \sum_{j=5,6} n_{ij}^1 \frac{S_{ij}}{S_{56}} \\ &\quad + \frac{n_{1234}^1 S_{12}}{S_{34}} + \frac{n_{1256}^1 S_{12}}{S_{56}} + \sum_{i=3,4,j=5,6} n_{12ij}^1 \frac{S_{12} S_{ij}}{S_{34} S_{56}}. \end{aligned} \quad (69)$$

In Eq. (69), the first five terms appear as a combination of IDoS^1 in bilayer systems, while the last term does not. For example, the fifth term comes from the bilayer between layer 1 and layer 2. In this case, the quasiperiodic pattern generated by primitive vectors a_3 and a_4 opens the energy gaps. In contrast, the last term with n_{12ij}^1 treats the energy gap that originates from the quasiperiodic pattern generated by primitive vectors a_i of layer 2 and a_j of layer 3, reflecting the trilayer nature. Combining IDoS for each layer, we obtain

$$\begin{aligned} &\left(\frac{1}{S_{12}} + \frac{1}{S_{34}} + \frac{1}{S_{56}} \right) \text{IDoS} \\ &= \frac{1}{S_{12}S_{34}S_{56}} \left[(n_\emptyset^1 + n_{3412}^2 + n_{5612}^3) S_{34}S_{56} \right. \\ &\quad + (n_{1234}^1 + n_\emptyset^2 + n_{5634}^3) S_{12}S_{56} \\ &\quad + (n_{1256}^1 + n_{3456}^2 + n_\emptyset^3) S_{12}S_{34} \\ &\quad + \sum_{i=1,2} \sum_{j=3,4} (n_{ij}^1 + n_{ij}^2 + n_{56ij}^3) S_{ij}S_{56} \\ &\quad + \sum_{i=1,2} \sum_{j=5,6} (n_{ij}^1 + n_{34ij}^2 + n_{ij}^3) S_{ij}S_{34} \\ &\quad \left. + \sum_{i=3,4} \sum_{j=5,6} (n_{12ij}^1 + n_{ij}^2 + n_{ij}^3) S_{ij}S_{12} \right]. \end{aligned} \quad (70)$$

Since labels such as $n_{ij}^1 + n_{ij}^2 + n_{56ij}^3$ appear only as a combination in the expression for the IDoS, we regard them as a single label. Therefore, redefining labels, we obtain

$$\text{IDoS} = \frac{\sum_{\substack{J \subset \{1,\dots,6\} \\ |J|=2}} n_J \frac{1}{S_J}}{\frac{1}{S_{12}} + \frac{1}{S_{34}} + \frac{1}{S_{56}}}, \quad (71)$$

where J labels a set of two integers from 1 to 6. The number of combinations to choose two integers J from 1 to 6 is 15. Thus to label a one-dimensional trilayer, we need 15 integers. In a similar manner, to label two-dimensional N -layer systems, we need to choose two vectors from $2N$ primitive vectors, which leads to ${}_{2N}C_2 = N(2N - 1)$ integers.

B. General D -dimensional N -layer systems

Similarly, we can also formulate the GLT in the D -dimensional N -layer MLTFs. The noncommutative parameter of the NCT for layer 1 is written as

$$\theta^1 = \begin{pmatrix} O & \Theta \\ -{}^t\Theta & O \end{pmatrix},$$

$$\Theta = \begin{pmatrix} (\mathbf{a}_1 \cdot \mathbf{b}_{D+1}) & \cdots & (\mathbf{a}_1 \cdot \mathbf{b}_{DN}) \\ \vdots & \ddots & \vdots \\ (\mathbf{a}_D \cdot \mathbf{b}_{D+1}) & \cdots & (\mathbf{a}_D \cdot \mathbf{b}_{DN}) \end{pmatrix}. \quad (72)$$

From this matrix, we choose submatrix θ_J^1 and calculate the Pfaffian. When $\dim \theta_J^1 = 2d$, a condition to obtain nonzero Pfaffian is to choose d indices from $1, \dots, D$ and d indices from $D+1, \dots, DN$. We denote chosen indices as $\mu \subset \{1, \dots, D\}$ and $\nu \subset \{D+1, \dots, DN\}$. Then, the Pfaffian of

the submatrix is given by

$$\text{Pf}(\theta_J^1) = \det \begin{pmatrix} (\mathbf{a}_{\mu_1} \cdot \mathbf{b}_{\nu_1}) & \cdots & (\mathbf{a}_{\mu_1} \cdot \mathbf{b}_{\nu_d}) \\ \vdots & \ddots & \vdots \\ (\mathbf{a}_{\mu_d} \cdot \mathbf{b}_{\nu_1}) & \cdots & (\mathbf{a}_{\mu_d} \cdot \mathbf{b}_{\nu_d}) \end{pmatrix}, \quad (73)$$

where $J = \mu \cup \nu$. When $d = D$, this simplifies to

$$\begin{aligned} \text{Pf}(\theta_J^1) &= \det \begin{pmatrix} (\mathbf{a}_{\mu_1} \cdot \mathbf{b}_{\nu_1}) & \cdots & (\mathbf{a}_{\mu_1} \cdot \mathbf{b}_{\nu_D}) \\ \vdots & \ddots & \vdots \\ (\mathbf{a}_{\mu_D} \cdot \mathbf{b}_{\nu_1}) & \cdots & (\mathbf{a}_{\mu_D} \cdot \mathbf{b}_{\nu_D}) \end{pmatrix} \\ &= \det \begin{pmatrix} - & \mathbf{a}_{\mu_1} & - \\ \vdots & \vdots & \vdots \\ - & \mathbf{a}_{\mu_D} & - \end{pmatrix} \det \begin{pmatrix} | & & | \\ \mathbf{b}_{\nu_1} & \cdots & \mathbf{b}_{\nu_D} \\ | & & | \end{pmatrix} \\ &= \frac{S_\mu}{S_\nu} = \frac{S^1}{S^1}. \end{aligned} \quad (74)$$

In the other cases, we obtain

$$\begin{aligned} \text{Pf}(\theta_J^1) &= \det \left[\begin{pmatrix} - & \mathbf{a}_{\mu_1} & - \\ \vdots & \vdots & \vdots \\ - & \mathbf{a}_{\mu_d} & - \end{pmatrix} \begin{pmatrix} | & & | \\ \mathbf{b}_{\nu_1} & \cdots & \mathbf{b}_{\nu_d} \\ | & & | \end{pmatrix} \right] \\ &= \det \left[\begin{pmatrix} - & \mathbf{a}_{\bar{\mu}_1} & - \\ \vdots & \vdots & \vdots \\ - & \mathbf{a}_{\bar{\mu}_{D-d}} & - \\ - & \mathbf{a}_{\mu_1} & - \\ \vdots & \vdots & \vdots \\ - & \mathbf{a}_{\mu_d} & - \end{pmatrix} \begin{pmatrix} | & & | & & | \\ \mathbf{b}_{\bar{\mu}_1} & \cdots & \mathbf{b}_{\bar{\mu}_{D-d}} & \mathbf{b}_{\nu_1} & \cdots & \mathbf{b}_{\nu_d} \\ | & & | & & | \end{pmatrix} \right] \\ &= (\pm 1) \frac{S^1}{S_{\bar{\mu}_1, \dots, \bar{\mu}_{D-d}, \nu_1, \dots, \nu_d}}. \end{aligned} \quad (75)$$

Here, $\mu \cup \bar{\mu} = \{1, \dots, D\}$, and ± 1 is the sign of the permutation of \mathbf{a}_i 's with $\{\bar{\mu}_1, \dots, \bar{\mu}_{D-d}, \mu_1, \dots, \mu_d\}$. This sign is not important to express IDoS, as we can get rid of it by redefining integer labels. Using the results above, the IDoS for layer 1 is expressed as

$$\text{IDoS}^1 = n_\emptyset^1 + \sum_{\substack{\mu \subset \{1, \dots, D\} \\ \nu \subset \{D+1, \dots, DN\} \\ |\mu \cup \nu| = D}} n_{\mu\nu}^1 \frac{S^1}{S_{\mu\nu}}. \quad (76)$$

In a similar manner, we can also calculate the IDoS for layer l . Using the relationship,

$$\left(\sum_l \frac{1}{S^l} \right) \text{IDoS} = \sum_l \frac{1}{S^l} \text{IDoS}^l, \quad (77)$$

we obtain the IDoS for the D -dimensional N -layer as

$$\text{IDoS} = \frac{\sum_{\substack{J \subset \{1, \dots, DN\} \\ |J| = D}} n_J \frac{1}{S_J}}{\sum_l \frac{1}{S^l}}. \quad (78)$$

This formula shows that the number of choices of J that have a nonzero contribution is ${}_D C_D$, which indicates that

we need ${}_D C_D$ integers to label the energy gap structure of D -dimensional N -layer MLTFs generally.

V. NUMERICAL CALCULATION

We demonstrate the validity of the obtained gap labels in the case of one-dimensional systems. First, we consider the bilayer system. We then move on to the trilayer system with large gaps between layers, which is ideal to project out the other layers into potentials.

First, we consider a bilayer consisting of layers with lattice constant 1 and θ . The Hamiltonian is composed of the two single-layer Hamiltonians with nearest-neighbor coupling and an interlayer coupling term:

$$\begin{aligned} \hat{H} &= \sum_{l=1,2} \sum_{n^l} [t^l |n^l + 1\rangle \langle n^l| + \text{H.c.}] \\ &\quad + \sum_{n^1, n^2} [V e^{-\gamma r(n^1, n^2)} |n^1\rangle \langle n^2| + \text{H.c.}]. \end{aligned} \quad (79)$$

Here $r(n^1, n^2)$ is the distance between sites n^1 and n^2 , which we define $r(n^1, n^2) = |n^1 a^1 - n^2 a^2|$, and we take $t^1 = 1, t^2 = 2, V = 5, \gamma = 10$. The result is shown in Fig. 3. The color

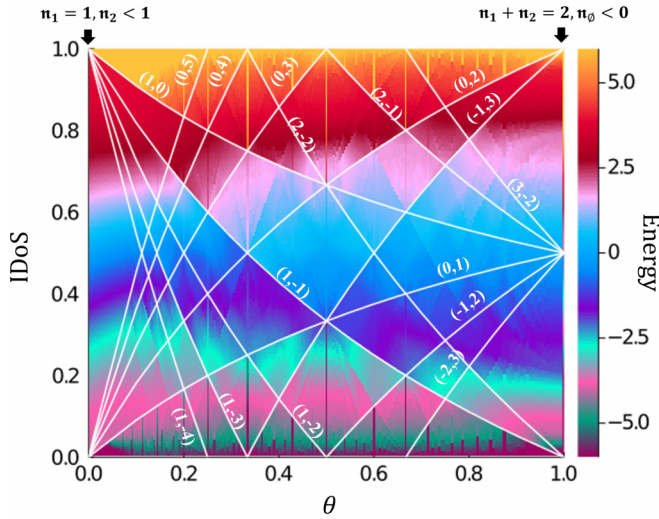


FIG. 3. The IDoS of the bilayer system against lattice constant θ . The color changes with energy. The region where the color changes sharply corresponds to the energy gap. White lines are energy gaps predicted by the GLT with labels (n_1, n_2) defined in Eq. (51). The labels of energy gaps whose IDoS is 1 at $\theta = 0$ satisfies $n_1 = 1$ and $n_2 < 1$. The labels of energy gaps whose IDoS is 1 at $\theta = 1$ satisfies $n_1 + n_2 = 2$ and $n_2 < 0$.

corresponds to the energy of eigenstates. The sharp color changes correspond to the energy gaps. The white solid curves are the position of the energy gap predicted from the generalized GLT in Eq. (51), where we indicate the associated integer labels. The white curves coincide with the position of the energy gap (where the color changes sharply), and they show that the generalized GLT holds in the present system. Vertical lines without a color change appear in fractional θ 's. While we show the curves associated with a few labels, we can also reproduce the positions of other energy gaps from the GLT as well. Next, we show numerical calculations in a trilayer system. Lattice constants are $a^1 = 1, a^2 = \alpha, a^3 = \alpha\beta$, and β is fixed to 12/13. The Hamiltonian is

$$\begin{aligned} \hat{H} = & \sum_{l=1}^3 \sum_{n^l} [t^l (|n^l + 1\rangle \langle n^l| + \text{H.c.}) + E^l |n^l\rangle \langle n^l|] \\ & + \sum_{n^1, n^2} [(V e^{-\gamma r(n^1, n^2)})^2 |n^1\rangle \langle n^2| + \text{H.c.}] \\ & + \sum_{n^2, n^3} [(V e^{-\gamma r(n^2, n^3)})^2 |n^2\rangle \langle n^3| + \text{H.c.}] \\ & + \sum_{n^3, n^1} [V e^{-\gamma r(n^3, n^1)} |n^3\rangle \langle n^1| + \text{H.c.}]. \end{aligned} \quad (80)$$

Here we take $t^1 = t^2 = t^3 = 2, V = 2, \xi = 2$. E^l 's are additional parameters to show the energy gap clearly, and we set $E^1 = 10, E^2 = 0, E^3 = -10$.

The energy spectrum under the PBC is shown in Fig. 4. Blue points are the energy spectrum, and red arrows show the energy gap predicted by the GLT. Among the energy gaps, there are two trivial gaps $(n_1, n_2, n_3) = (0, 0, 1)$ and $(0, 1, 1)$. $(0, 0, 1)$ corresponds to filling layer 3 only, and $(0, 1, 1)$ corresponds to filling layers 2 and 3. These gaps open without

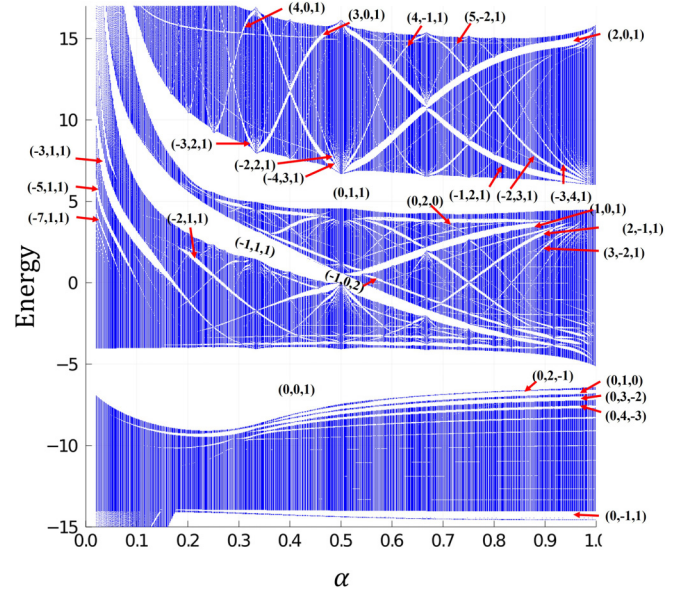


FIG. 4. Trilayer model with large gaps. Here, we set $\beta = 12/13$. Parameters are $t_1 = t_2 = t_3 = 2, V = 2, \xi = 2, E_1 = 10, E_2 = 0, E_3 = -10$. Blue points are the energy spectrum, and red lines are the energy gap predicted by the GLT. Arrows indicate the energy gap, and their labels (n_1, n_2, n_3) .

quasiperiodicity, so they are stable against the change of α . In Fig. 4, the sizes of the energy gaps are different. This is due to the exponential decay of the interlayer coupling. When the interlayer coupling takes a large value, on the Bragg lines the energy gap is also large. Even in the case in which the energy gaps are small, e.g., $(5, -2, 1)$, we can also label energy gaps. Therefore, we can also predict energy gaps in the trilayer systems using GLT.

We note the limitations for the choices of E^l . In this calculation, we added energy offsets to separate the energy bands of the three layers. This allows us to focus on intraband energy gaps that can be captured by the GLT. When energy bands are energetically close and hybridized with each other, interband energy gaps appear that are not necessarily captured by the GLT. Characterization of those interband energy gaps remains a future problem.

VI. DISCUSSIONS

In this paper, we have extended the GLT to MLTFs using the approach from the noncommutative torus, which allows us to treat all layers on an equal footing. We derived the GLT for general D -dimensional N -layer systems by combining previous results on the GLT [19,32] and redefinition of the normalized trace for each layer using a continued fraction and the inductive limit. As a result, we have obtained the general expression of IDoS in Eq. (78), and we found that the number of gap labels is generally given by $D_N C_D$. In addition, the obtained GLT formula was found to be consistent with the result from the SCN approach. The present NCT approach also gives a reinterpretation of the result obtained from the SCN approach. (For details, see Appendix).

We note the validity of treating the interlayer coupling as an effective quasiperiodic intralayer coupling for each layer. In this paper, we focused on the situation in which we can treat the interlayer coupling as an effective intralayer coupling for each layer. This is a good approximation when the energy bands from different layers are energetically separated. When the states from different layers are energetically close and hybridized due to the interlayer coupling, the resulting energy gaps do not arise from the quasiperiodicity, and they are not expected to be characterized by the GLT. To be more precise, it is not evident whether one can rewrite the Hamiltonian with general interlayer couplings as an operator belonging to a NC torus without projecting to the effective intralayer coupling.

An interesting future direction will be studying the relationship between the GLT and the flat bands in the MLTFs. In MLTFs such as twisted bilayer graphene, an emergence of flat bands at certain angles has been reported. This is a consequence of the gap opening between replicas of the energy band, and it originates from the quasiperiodicity. Recently, the flat band in twisted bilayer graphene has been studied using Jacobi θ functions [33–35], where one can define a commutation relationship for quasiperiodic functions in a similar manner to those for S and U used in Sec. III [36]. One can interpret that the θ functions are describing the wave functions of quasiperiodic systems, while the NC torus is describing the Hamiltonian. Thus, the GLT may also be useful to study the flat bands in quasiperiodic systems if a relationship between the GLT and the θ function is established.

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APPENDIX: SLIDING CHERN NUMBER

In MLTFs, a new topological index that comes from the sliding of two-dimensional layers was proposed independently in Refs. [20,37,38]. Here, we call it the sliding Chern number (SCN) following Ref. [20].

1. Gedanken experiment to relate SCN and gap labels

In Ref. [20], a gedanken experiment was conducted to clarify the relationship between the SCN and a quantized charge transport. This argument can be used to obtain GLT for one-dimensional bilayer systems with an extension.

We consider a one-dimensional bilayer system without the internal degree of freedom. The lattice constant of the bottom layer is 1 and the top layer is p/q . Here, p and q are coprime to each other, and two layers are connected through interlayer coupling.

In this case, we can define the moiré unit cell for the bilayer system and its lattice constant to be q .

When we slide the top layer by q , the system before and after the sliding is identical, yet electrons on the top layer are transferred. With the constraint that the system must be identical in two cases, the number of transferred electrons is a multiple of sites inside the moiré unit cell, $n_t q$ ($n_t \in \mathbb{Z}$).

In a similar manner, we can also slide the bottom layer by q into the opposite direction. In this case, the number of transferred electrons is a multiple of $n_b p$ ($n_b \in \mathbb{Z}$).

Since two slid bilayers are related through the translation of the entire system by q . We can obtain the following equation:

$$n_t q = n_b p + N. \quad (\text{A1})$$

Here, N is the number of electrons inside the moiré unit cell. In Ref. [20], it was shown that n_t and n_b are the sliding Chern number.

To see the relationship of the above argument with the IDoS, we divide both sides with the system size $p + q$, which leads to

$$\text{IDoS} = n_t \frac{q}{p+q} - n_b \frac{p}{p+q}. \quad (\text{A2})$$

From the definition, IDoS is the number of electrons divided by the system size $N/(p+q)$. Finally, we take the incommensurate limit. Replacing p/q with an irrational number θ , we obtain

$$\text{IDoS} = \frac{n_t - n_b \theta}{1 + \theta}. \quad (\text{A3})$$

Therefore, we can also relate the SCN with IDoS. This gedanken experiment does not depend on the detail of the Hamiltonian, and Eq. (A3) coincides with the result in Sec. III.

2. Two and higher dimensions

In Ref. [31], the relationship between the energy gaps of hBN/graphene/hBN trilayer heterostructure and integer labels were pointed out, and later the authors studied the relationship between the energy gap structure and the integer labels in general two-dimensional multilayer systems in Ref. [21]. From these studies, they derived the following expression for the IDoS:

$$\text{IDoS}(G) = n_0 + \sum_{i=1,2} \sum_{j=3,4} n_{ij} \frac{S_{ij}}{S_{12}} + n_{1234} \frac{S_{34}}{S_{12}}, \quad (\text{A4})$$

which is consistent with the generalized GLT formula for the $D = 2, N = 2$ case. More recently, Yamamoto and Koshino pointed out that one can label energy gaps of the three-dimensional system under incommensurate potential with the third Chern number [39]. This is consistent with our result of the generalized GLT, in that we can transform the Hamiltonian of a D -dimensional lattice under incommensurate potential to an NC 2D torus, and the top Chern number is the D th Chern number [40].

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