

Topological charge pumping by a sliding moiré pattern

Manato Fujimoto¹,¹ Henri Koschke^{1,2},^{1,2} and Mikito Koshino¹

¹*Department of Physics, Osaka University, Osaka 560-0043, Japan*

²*Department of Physics, University of Cologne, 50923 Cologne, Germany*



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We study the adiabatic topological charge pumping driven by interlayer sliding in the moiré superlattices. We show that, when we slide a single layer of the twisted bilayer system relatively to the other, a moiré pattern flow and a quantized transport of electrons occur. The number of pumped charges is quantized to a sliding Chern number, which is related to the interlayer sliding degree of freedom. In the twisted bilayer graphene, the topological pumping current flows perpendicularly to the sliding direction when the Fermi energy is in the energy gap above or below the nearly-flat bands.

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The spiral pump, also known as the Archimedes' screw, is a mechanical device to pump up water by a rotating spiral blade. The machine converts the cyclic motion of blade to a directed motion of water, and it works no matter how slowly the screw is rotated. The quantum version of this phenomena is known as the Thouless pumping [1], where an adiabatic, cyclic movement of a periodic potential pumps particles without a bias voltage. The amount of the transferred particles is precisely quantized and expressed as a topological invariant. The experimental realization of quantum pumping requires precise control of the time-dependent periodic potential. The electron pumping experiments have been performed in various semiconductor-based nanoscale devices [2–4]. More recently, the topological charge pump was realized in ultracold atoms in optical superlattices [5–7], and it was also extensively studied in theory [8–15].

In this Rapid Communication, we propose a simple realization of topological pumping using the moiré superlattice of the two-dimensional (2D) materials. When two periodic lattices are overlaid on top of each other with a relative rotation, the lattice mismatch between the layers gives rise to a moiré interference pattern. If we slide a single layer of the twisted bilayer system relatively to the other, the moiré pattern flows at a much faster speed than the sliding speed as shown in Fig. 1. The process is cyclic, as sliding by a single atomic constant shifts the moiré pattern exactly by a single superlattice period. We can then ask how the electrons are transported by the movement of the moiré pattern.

Here we study the topological charge pumping driven by interlayer sliding in the moiré superlattices. We first consider a one-dimensional (1D) double-chain model composed of two tight-binding chains with different lattice constants. We show that the number of pumped charges in the interlayer sliding process is quantized into a sliding Chern number, which satisfies a Diophantine equation similar to that for the quantum Hall effect [16]. We apply the same argument to the twisted bilayer graphene (TBG) [17–23], and find that eight Chern numbers are associated with each single gap, which correspond to different pumping directions under different sliding directions. In low-angle twisted bilayer graphenes,

we show that energy gaps above and below the nearly-flat bands [22,24] has nonzero sliding Chern numbers. When the Fermi energy is in either of those gaps, the electrons are pumped almost perpendicularly to the sliding direction following the movement of the moiré pattern.

Let us consider a 1D double chain as illustrated in Fig. 2(a). The system contains two atomic chains with different lattice constants, which are arranged parallel to one another in a certain distance d_0 . The chains are denoted by 1 and 2 and their lattice constants by a_1 and a_2 , respectively. In the following, we consider a commensurate case $N_1 a_1 = N_2 a_2 = L$ with integers N_1 and N_2 , where a vertical overlap of an atom pair from both chains appears in a period L .

We calculate the eigenenergies and eigenfunctions in a double-chain tight-binding model with s atomic orbitals on each single site. The Hamiltonian is written as

$$H = - \sum_{\langle i,j \rangle} t(\mathbf{R}_i - \mathbf{R}_j) |\mathbf{R}_i\rangle \langle \mathbf{R}_j| + \text{H.c.}, \quad (1)$$

where \mathbf{R}_i and $|\mathbf{R}_i\rangle$ represent the lattice point and the atomic state at site i , respectively, and $t(\mathbf{R}_i - \mathbf{R}_j)$ is the transfer integral between site i and site j . For the intrachain hopping we just take the nearest-neighbor hopping and it is assumed to be the same for both chains and defined as unit of energy. For the hopping between sites on the different chains, we assume $t(d) = t_0 e^{-(d-d_0)/\delta_0}$ where $d = |\mathbf{R}_i - \mathbf{R}_j|$ and δ_0 is decay length. In this Rapid Communication we assume $t_0 = 4.0$, $d_0 = 1.0$, and $\delta_0 = 0.1$.

We consider an adiabatic charge pumping caused by a relative sliding of chains. By starting from an initial state in Fig. 2(a), we horizontally shift either of chain $l = 1$ or 2 by λa_l ($0 \leq \lambda \leq 1$) with the other chain fixed. When λ is increased from 0 to 1, the Hamiltonian returns to its original state. We assume that the shift occurs in a sufficiently long time, so that we can treat the problem as an adiabatic topological pumping [1]. The charge transport in such a process is expressed as a change of the polarization. If the Fermi energy lies inside a certain gap of the spectrum, the electric polarization, or the center of mass of the occupied electrons,

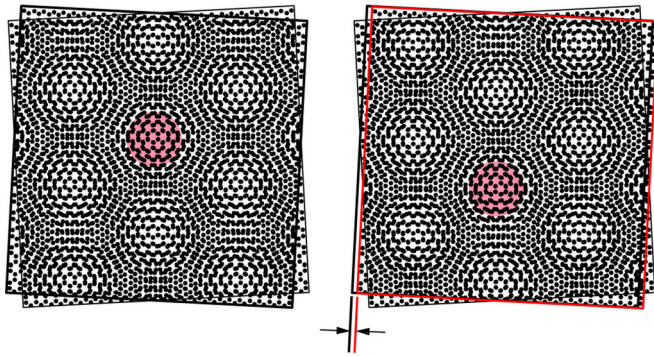


FIG. 1. Moiré pumping in twisted bilayer graphene. From left to right, we slide the layer 1 by half of the atomic constant and then the moiré pattern shifts by the half of the moiré period as indicated by a pink circle.

is given by

$$P(\lambda) = \sum_{n \in \text{occ.}} \frac{L}{2\pi} \int_{-\pi/L}^{\pi/L} dk i \langle u_{nk}(\lambda) | \frac{\partial}{\partial k} | u_{nk}(\lambda) \rangle, \quad (2)$$

where $u_{nk}(\lambda)$ is the Bloch eigenstate of the n th band in the instantaneous Hamiltonian at shift λ , and occ. represents the occupied bands below the Fermi energy. The charge transport during the process is then given by $\Delta P = \int_0^1 d\lambda (\partial P / \partial \lambda)$. This is expressed as $\Delta P = CL$ with the sliding Chern number,

$$C = \sum_{n \in \text{occ.}} \frac{iL}{2\pi} \int_{-\pi/L}^{\pi/L} dk \int_0^1 d\lambda \left[\left\langle \frac{\partial u}{\partial \lambda} \middle| \frac{\partial u}{\partial k} \right\rangle - \left\langle \frac{\partial u}{\partial k} \middle| \frac{\partial u}{\partial \lambda} \right\rangle \right], \quad (3)$$

where $u = u_{nk}(\lambda)$. We can define two different Chern numbers C_l ($l = 1, 2$) for the movement of chain l .

Figure 2(b) shows the evolution of a wave function of the lowest band in the double chain of $(N_1, N_2) = (10, 11)$, where the chain 2 (red) is shifted by λa_2 with the chain 1 (blue) fixed.

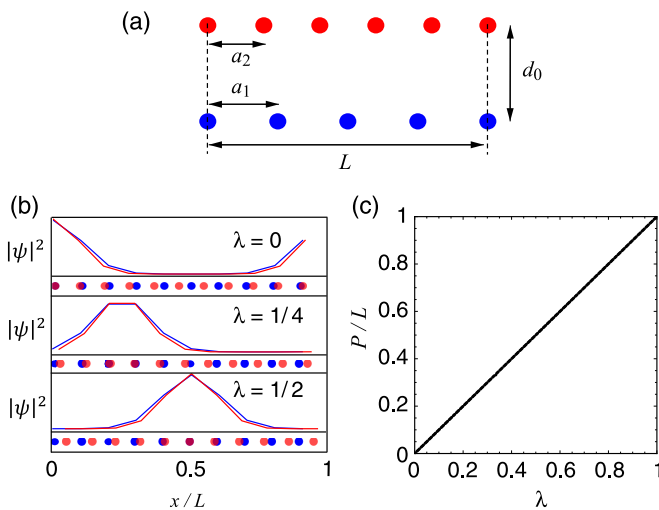


FIG. 2. (a) Double-chain model with $N_1 = 4, N_2 = 5$. (b) Evolution of a wave function of the lowest band in the double chain of $(N_1, N_2) = (10, 11)$, where the chain 2 (red) is shifted by λa_2 with the chain 1 (blue) fixed. (c) Polarization P [Eq. (2)] in the lowest gap as a function of sliding parameter λ .

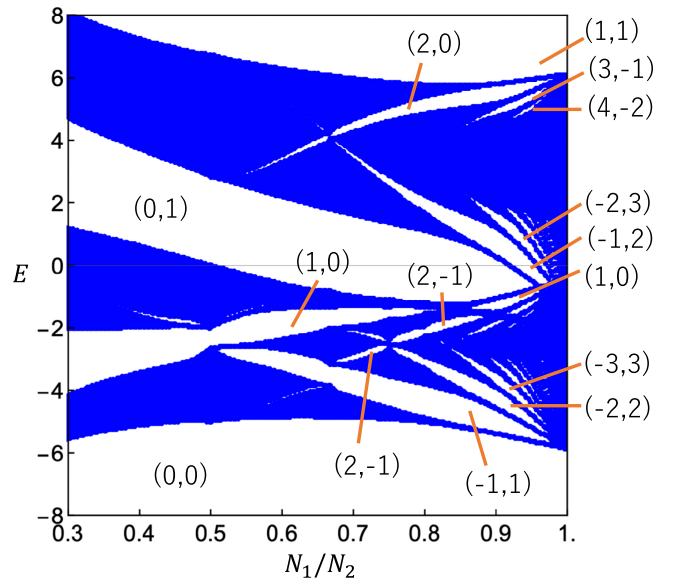


FIG. 3. Energy spectrum of the one-dimensional double-chain model as a function of N_1/N_2 . The numbers assigned to gaps indicate the sliding Chern numbers (C_1, C_2) .

The blue and red dots in the bottom represent the horizontal positions of chains 1 and 2, respectively. We see that the wave center exactly follows the atom overlap region, i.e., the region where the chain 1 atoms and chain 2 atoms are overlapping in the horizontal position. In this particular system ($N_2 - N_1 = 1$), the center of the overlap region is given by $x = \lambda L$ as a function of sliding parameter λ , so it moves exactly by the superlattice period L from $\lambda = 0$ to 1. In Fig. 2(c), we plot the polarization P [Eq. (2)] in the lowest gap as a function of shift λ , where we actually see that the charge is pumped by L after one cycle, i.e., $C_2 = 1$. We can consider a similar process to move chain 1 by fixing chain 2 instead, and then we have $C_1 = -1$, i.e., the change is pumped by a single moiré period in the negative direction.

We calculate the band structure and the sliding Chern numbers for various configurations of N_1 and N_2 . In Fig. 3, we plot the energy spectrum as a function of N_1/N_2 , where the filled area represents the energy region where the eigenstates exist, and the numbers assigned to the gaps are the sliding Chern numbers (C_1, C_2) . The picture shows some similarities with Hofstadter's butterfly [25] with the quantized Hall integers in a two-dimensional periodic system under the magnetic field [16]. Actually the sliding Chern numbers can be found by using a Diophantine equation similar to that in the quantum Hall systems [16], without integrating the Berry curvature in Eq. (3), as in the following manner.

Let us consider a double chain specified by N_1 and N_2 , and assume the Fermi energy lies in a gap with r bands below, i.e., r bands out of $N_1 + N_2$ bands in total are fully occupied. If we fix chain 2 and shift chain 1 by $L (= N_1 a_1)$, the number of pumped electrons is given by $N_1 C_1$, i.e., $N_1 C_1$ electrons passed through any cross section perpendicular to the double chain. On the other hand, if we fix chain 1 and shift chain 2 by $-L (= -N_2 a_2)$, the number of pumped electrons is given by $-N_2 C_2$, i.e., $N_2 C_2$ electrons passed in the negative direction. The former and the latter processes share the same relative

motion between the two chains, but differ only in the absolute position of the final state by L . If we shift the whole system (chains 1 and 2 together) by L following the latter process, it causes a pump of extra r electrons, because the number of electrons per a superlattice period L is equal to the number of occupied bands, r . The equality of the two processes leads to $N_1 C_1 = -N_2 C_2 + r$, or

$$N_1 C_1 + N_2 C_2 = r, \quad (4)$$

which is a Diophantine equation for the sliding Chern numbers.

If we define the ratio of the double periods as $\alpha = N_1/N_2 = a_2/a_1$ and the electron density as $\rho = r/N_2$, we have $\rho = C_1\alpha + C_2$. Now the Chern numbers C_1 and C_2 can easily be derived from the diagram of Fig. 3, by counting the number of states below a particular gap as a function of α , and calculating $\partial\rho/\partial\alpha$. This is an analog to Stréda's formula in the integer quantum Hall effect [26].

We can calculate the charge pumping in sliding TBGs in the same manner. We define the structure of TBG of twist angle θ by rotating layers 1 and 2 of the AA-stacked bilayer around a center of hexagon by $-\theta/2$ and $+\theta/2$, respectively. The lattice vectors of layer l are given by $\mathbf{a}_i^{(l)} = R(\mp\theta/2)\mathbf{a}_i$ with \mp for $l = 1, 2$, respectively, where $\mathbf{a}_1 = a(1, 0)$ and $\mathbf{a}_2 = a(1/2, \sqrt{3}/2)$ are the lattice vectors of the AA-stacked bilayer before the rotation, $a \approx 0.246$ nm is the lattice constant, and $R(\theta)$ represents the rotation by θ . When the rotation angle is small, the mismatch between the lattice vectors of the two layers gives rise to a long-range moiré pattern which is ruled by the primitive lattice vectors [27],

$$\mathbf{L}_i^M = [R(\theta/2) - R(-\theta/2)]^{-1}\mathbf{a}_i \quad (i = 1, 2). \quad (5)$$

The atomic structure of TBG is not exactly periodic in general, because the moiré period is generally incommensurate with the underlying atomic lattice. A commensurate structure with an exact period takes place when the twist angle θ coincides with the angle between $\mathbf{v}_1 = m\mathbf{a}_1 + n\mathbf{a}_2$ and $\mathbf{v}_2 = n\mathbf{a}_1 + m\mathbf{a}_2$ with certain integers m and n . Then the lattice points \mathbf{v}_1 on layer 1 and \mathbf{v}_2 on layer 2 of the nonrotated bilayer graphene merge after the rotation and a rigorously periodic structure is obtained. A lattice vector of the superlattice unit cell is then given by $\mathbf{L} = m\mathbf{a}_1^{(1)} + n\mathbf{a}_2^{(1)} = n\mathbf{a}_1^{(2)} + m\mathbf{a}_2^{(2)}$. The twist angle θ is equal to the angle between \mathbf{v}_1 and \mathbf{v}_2 , which is $\cos\theta = (1/2)(m^2 + n^2 + 4mn)/(m^2 + n^2 + mn)$. The 60° rotation of \mathbf{L} also gives a lattice vector because of C_6 rotational symmetry. We can choose two primitive lattice vectors as $\mathbf{L}_1 = R(-2\pi/3)\mathbf{L}$ and $\mathbf{L}_2 = R(-\pi/3)\mathbf{L}$, which can be written as

$$\begin{aligned} \mathbf{L}_1 &= n\mathbf{a}_1^{(1)} - (m+n)\mathbf{a}_2^{(1)} = m\mathbf{a}_1^{(2)} - (m+n)\mathbf{a}_2^{(2)}, \\ \mathbf{L}_2 &= (m+n)\mathbf{a}_1^{(1)} - m\mathbf{a}_2^{(1)} = (m+n)\mathbf{a}_1^{(2)} - n\mathbf{a}_2^{(2)}. \end{aligned} \quad (6)$$

In this choice, the rigorous period and the moiré period are simply related by $\mathbf{L}_i = |m-n|\mathbf{L}_i^M$ [27].

Now let us consider the charge pumping of a commensurate TBG. We adiabatically slide the layer l ($l=1$ or 2) by its own lattice period $\mathbf{a}_i^{(l)}$ ($i=1$ or 2) while the other layer is

fixed. The variation of polarization in this process is written as

$$\Delta\mathbf{P} = C_{i1}^{(l)}\mathbf{L}_1 + C_{i2}^{(l)}\mathbf{L}_2, \quad (7)$$

$$\begin{aligned} C_{ij}^{(l)} &= \sum_{n=\text{occ.}} \frac{iS}{(2\pi)^2} \int_{\text{BZ}} d^2k \int_0^1 d\lambda_i \\ &\times \left[\left\langle \frac{\partial u}{\partial \lambda_i} \middle| \frac{\partial u}{\partial k_j} \right\rangle - \left\langle \frac{\partial u}{\partial k_j} \middle| \frac{\partial u}{\partial \lambda_i} \right\rangle \right], \end{aligned} \quad (8)$$

where $u = u_{n\mathbf{k}}(\lambda_1, \lambda_2)$ is the Bloch eigenstate in the instantaneous Hamiltonian with the layer l shifted by $\lambda_1\mathbf{a}_1^{(l)} + \lambda_2\mathbf{a}_2^{(l)}$, BZ represents the first superlattice Brillouin zone, and $S = |\mathbf{L}_1 \times \mathbf{L}_2|$ is the superlattice unit cell area. $\partial/\partial k_j = (\mathbf{G}_j/|\mathbf{G}_j|) \cdot \nabla_{\mathbf{k}}$, and \mathbf{G}_j is the reciprocal lattice vectors satisfying $\mathbf{G}_j \cdot \mathbf{L}_j = 2\pi\delta_{ij}$. The sliding Chern number $C_{ij}^{(l)}$ represents the number of electrons passed through the unit-cell side perpendicular to \mathbf{G}_j (i.e., the cross section spanned by \mathbf{L}_2 for $j=1$, and \mathbf{L}_1 for $j=2$), during an adiabatic sliding of the layer l by $\mathbf{a}_i^{(l)}$. It is formally similar to, but different from the Chern number for the quantized Hall conductivity [16], as it is related to derivative in mechanical interlayer shift.

To obtain the Diophantine equation for the sliding Chern numbers in the TBG, we follow the same steps as in 1D. We assume that the Fermi energy is in a gap and r bands are fully occupied. Considering that a shift of layer 1 by $\mathbf{L}_1 [= n\mathbf{a}_1^{(1)} - (m+n)\mathbf{a}_2^{(1)}]$ is equivalent to a shift of layer 2 by $-\mathbf{L}_1 [= -m\mathbf{a}_1^{(2)} + (m+n)\mathbf{a}_2^{(2)}]$ followed by a shift of whole system by \mathbf{L}_1 , we obtain

$$\begin{aligned} nC_{11}^{(1)} + mC_{11}^{(2)} - (m+n)(C_{21}^{(1)} + C_{21}^{(2)}) &= r, \\ nC_{12}^{(1)} + mC_{12}^{(2)} - (m+n)(C_{22}^{(1)} + C_{22}^{(2)}) &= 0. \end{aligned} \quad (9)$$

A similar argument for the shift by \mathbf{L}_2 gives

$$\begin{aligned} (m+n)(C_{11}^{(1)} + C_{11}^{(2)}) - mC_{21}^{(1)} - nC_{21}^{(2)} &= 0, \\ (m+n)(C_{12}^{(1)} + C_{12}^{(2)}) - mC_{22}^{(1)} - nC_{22}^{(2)} &= r. \end{aligned} \quad (10)$$

The exact lattice commensurability is not actually important in low twist angles, where the physical property is approximately described by the continuum model, which is periodic in the moiré period \mathbf{L}_j^M [17,22,23,27–31]. Indeed, Eqs. (9) and (10) can also be transformed in a continuous form as follows. Since the rigorous period \mathbf{L}_j is $|m-n|$ times as large as the moiré period \mathbf{L}_j^M , a single continuum band corresponds to $|m-n|^2$ rigorous bands considering the zone folding, and therefore the number of occupied continuum bands is given by $\tilde{r} = r/|m-n|^2$. We can also define $\tilde{C}_{ij}^{(l)} = C_{ij}^{(l)}/|m-n|$ as the number of electrons passed through the cross section spanned by \mathbf{L}_j^M in the adiabatic sliding of the layer l by $\mathbf{a}_i^{(l)}$. Then Eqs. (9) and (10) become

$$\begin{aligned} \frac{\beta+1}{2}\tilde{C}_{11}^{(1)} + \frac{\beta-1}{2}\tilde{C}_{11}^{(2)} - \beta(\tilde{C}_{21}^{(1)} + \tilde{C}_{21}^{(2)}) &= \tilde{r}, \\ \frac{\beta+1}{2}\tilde{C}_{12}^{(1)} + \frac{\beta-1}{2}\tilde{C}_{12}^{(2)} - \beta(\tilde{C}_{22}^{(1)} + \tilde{C}_{22}^{(2)}) &= 0, \\ \beta(\tilde{C}_{11}^{(1)} + \tilde{C}_{11}^{(2)}) - \frac{\beta-1}{2}\tilde{C}_{21}^{(1)} - \frac{\beta+1}{2}\tilde{C}_{21}^{(2)} &= 0, \\ \beta(\tilde{C}_{12}^{(1)} + \tilde{C}_{12}^{(2)}) - \frac{\beta-1}{2}\tilde{C}_{22}^{(1)} - \frac{\beta+1}{2}\tilde{C}_{22}^{(2)} &= \tilde{r}, \end{aligned} \quad (11)$$

where $\beta = (1/\sqrt{3}) \cot(\theta/2)$.

In the TBGs with low-angle angles, it is known that the nearly-flat bands around the charge neutral point are separated from the rest of the spectrum by energy gaps [32–36]. If we assume that the Fermi energy lies in the gap just above the flat band, for example, we have $\tilde{r} = 4$ (relative to the charge neutral) by including the spin and valley degeneracies. The set of equations of Eq. (11) can be regarded as identities for a variable β , as it stands for any θ 's in the low-angle regime. Then the Chern numbers are uniquely determined as $\tilde{C}_{11}^{(1)} = \tilde{C}_{22}^{(1)} = 4$, $\tilde{C}_{11}^{(2)} = \tilde{C}_{22}^{(2)} = -4$, and otherwise 0. Actually, we can show that sliding the layer l by $\mathbf{a}_i^{(l)}$ leads to the moiré-pattern movement by $\pm \mathbf{L}_i^M$ with \pm for $l = 1, 2$, respectively. The above solution of $\tilde{C}_{ij}^{(l)}$ means that four electrons trapped at each AA-stacking region precisely follow the movement of the moiré pattern, as naturally expected.

To conclude, we studied the topological charge pumping driven by interlayer sliding in the moiré superlattices. The number of pumped charges is quantized to the sliding Chern numbers, which can be found as a solution of a Diophantine equation. When the Fermi energy is in the energy gap above or below the nearly-flat bands of the twisted bilayer graphene,

four electrons per superlattice period are conveyed following the flow of the moiré pattern perpendicularly to the sliding direction. The interlayer sliding in moiré superlattices is, in principle, experimentally feasible by using a mechanical device [37]. We expect that the slide-driven topological pumping may be observed as an electric current by source and drain electrodes appropriately attached. If the system is isolated, the interlayer sliding should generate an electric polarization by accumulated charge at the edge. This naturally implies the existence of the edge states in the energy gap with nonzero sliding Chern numbers. The bulk-edge correspondence of this problem will be studied elsewhere. Also, the topological pumping in other moiré bilayer systems, such as graphene/hBN [38–46] and transition metal dichalcogenide bilayers [47–52], is left for future work.

Note added. Recently, we became aware of preprints which also report the topological pumping by a sliding moiré pattern [53,54].

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