Two-Dimensional Thouless Pumping of Ultracold Fermions in Obliquely Introduced Optical Superlattice

Fuyuki Matsuda, Masaki Tezuka, and Norio Kawakami*
Department of Physics, Kyoto University, Kyoto 606-8502, Japan
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We propose a two-dimensional (2D) version of Thouless pumping which can be realized by using ultracold atoms in optical lattices. To be specific, we consider a 2D square lattice tight-binding model with obliquely introduced superlattice. We show that quantized particle transport occurs in this system, and that the transport is expressed as a solution of a Diophantine equation. This topological nature can be understood easily by mapping the Hamiltonian onto a 3D cubic lattice model with a homogeneous magnetic field. On the other hand, in the weak potential limit, we uncover that the pumping direction is restricted exactly to an x-axis or a y-axis direction. This difference in two limits causes a topological transition. Furthermore, we demonstrate by numerical simulation that the above phenomena are measurable in cold atom systems.

I. INTRODUCTION

The studies of quantum Hall effect opened up a wide research area which is known as topological phases [1, 2]. Topological phases are characterized by the associated invariants, which are prohibited to vary unless the energy gap closes. Moreover, topological phases have a characteristic property called bulk-edge correspondence, which guarantees the existence of the edge states, meaning that electrons can only move on the edge of a given material, as far as the bulk topological invariant has a non-trivial value. In quantum Hall systems, the topological invariant is defined by the Chern number, and it appears as the quantized Hall conductance. Thouless et al. showed that this Chern number satisfies a certain Diophantine equation [3]. Similar relationships also appear in 3D quantum Hall systems [4–6].

Topological phases can be realized in various experimental platforms, not only in materials, but also in optical waveguides [7], photonic systems [8–10], etc. In particular, great efforts have been made to realize topological insulators in cold atom systems by using synthetic gauge fields, which are induced by an optical lattice [11]. Various topological systems have been realized in cold atom systems, for instance, Su-Schriefer-Heeger model [12], Hofstadter model [13, 14], Synthetic dimensions [15, 16], and Haldane model [17]. Recently, topological charge pumping which is called Thouless pumping [18, 19] has been realized in cold atom systems [20, 21], and also many theoretical proposals have been made in numerous studies [22–30].

Mapping Hamiltonian between different dimensions plays an important role in understanding physical properties. One of the significant examples of mapping can be seen in the problem of Hofstadter butterfly [31]. Hofstadter mapped a two-dimensional (2D) system of square lattice under a uniform magnetic field into a 1D equation, which is called the Harper equation. Interestingly, a recent research of adiabatic pumping used this mapping backwards, and showed the topological equivalence over a certain group of Hamiltonians. This kind of mapping into higher dimensions can be applied not only to 1D systems, but also to two and higher dimensional systems [32].

In this paper, we consider a 2D tight-binding model of particles that hop on a square lattice in the presence of modulation in the on-site potential and the hopping amplitude, where the modulation amplitude depends only on the distance from an inclined line. We find that this model has topological nature. First, we show that edge-localized states appear when a strong binding potential which constrains particle around an inclined line exists. Also, if we pay our attention to the energy spectrum, these edge states cross the bulk energy band gap. These topological insulator-like behaviors can be understood clearly when we apply a mapping from higher dimensions to this 2D system. In a 3D mapped Hamiltonian, a set of weak Chern numbers of this system becomes non-zero when the chemical potential is controlled adequately, which implies that this system is a weak topological insulator. These weak Chern numbers determine the adiabatic pumping in the original 2D system.

This paper is organized as follows. In section II, we introduce a 2D square lattice tight-binding model with an obliquely introduced potential in order to investigate the effect of the superimposed potential in the context of topological phases. The existence of edge-localized states and band-crossing states, which are typical phenomena in topological phases, are shown. Also, we show that the Hofstadter butterfly structure appears in our model. In section III, we consider a continuum model in order to consider the above tight-binding model and treat it more precisely. We focus on two limits: weak superlattice and strong superlattice limit, which we call the Hofstadter regime and the sliding regime. In the Hofstadter regime, the amount of the charge pumping corresponds to the solution of the Diophantine equation. In the sliding limit, the pumping behavior completely changes to “rectified pumping”, in which a pumping direction is restricted to exactly x-direction or exactly y-direction. In section IV, we conclude our paper.
II. TOPOLOGICAL ASPECTS IN 2D OPTICAL LATTICE WITH OBLIQUELY INTRODUCED POTENTIAL

A. Model

Recently, the development of experimental techniques regarding cold atoms in optical lattice is remarkable, and the degree of freedom in designing the quantum simulation is high. Triangle lattice, square lattice, and hexagonal lattice have all been realized in cold atom systems. Moreover, it is possible to realize non-standard lattices in cold atom systems. One example of such lattices is the lattice made by superimposing a usual lattice potential and a superlattice potential. For example, in Ref.33, Taie et al. realized an optical Lieb lattice by adding a diagonal lattice to a usual square optical lattice.

Also, this paper is partly motivated by recent remarkable progress in solid state, i.e. twisted bilayer graphene. Twisted bilayer graphene, which is receiving a lot of attention lately because of the realization of unconventional superconductivity[34]. Twisted bilayer graphene has been investigated in many contexts, such as its electronic structures[35, 36], flat bands[37], topological band structures[38], and Moiré butterflies[39]. It provides also a prototypical example of superimposed lattice potential.

Stimulated by the above mentioned previous studies, it is natural to ask what happens if the additional diagonal lattice in the optical Lieb lattice is twisted. Now, we consider a fermion gas loaded in the 2D optical square lattice with a superlattice structure which is introduced obliquely. We study the ground-state properties of the system which is described by the following hamiltonian:

\[ \hat{H} = \sum_{m,n} \left[ -t \left( \hat{c}_{m+1,n}^{\dagger} \hat{c}_{m,n} + \hat{c}_{m,n+1}^{\dagger} \hat{c}_{m,n} \right) + \text{H.c.} \right] + \sum_{m,n} \left[ V_{m,n} \hat{c}_{m,n}^{\dagger} \hat{c}_{m,n} \right] \]

\[ V_{m,n} = V(m + \alpha n - \delta) \]

where \( \hat{c}_{m,n}^{\dagger}(\hat{c}_{m,n}) \) is the fermion creation (annihilation) operator, \( t \) is the hopping strength, \( \delta \) is the parameter of the real space potential shift, and \( \alpha \) is the tangent of the superlattice. The boundary conditions are taken both open and periodic.

B. Obliquely introduced single well

First, we consider the case of \( \alpha = (\sqrt{5} + 1)/2 \approx 1.618 \) with open boundary conditions. We take \( V(x) = -V e^{-x^2/w^2} \) as an oblique linear-shaped potential, which restricts particles to move around the potential in the low-energy region. On-site potential in this system is plotted in Fig. 1. As a consequence of the overlap of the square lattice and obliquely introduced potential, this model can be effectively considered as a 1D tight binding model with a superlattice. This effective superlattice opens the energy gap. By the analogy to the previous study of topological aspects of 1D superlattice, the edge states seem to appear when we drive the phase of the superlattice, which corresponds to the parameter \( \delta \) in this model. We can see the existence of band-crossing states in the energy spectrum as a function of \( \delta \) in Fig. 2. Note that the bulk band is fixed because we choose an irrational number for tangent \( \alpha \).

By changing \( \alpha \), the distribution of energy band will also changes. Fig. 4 shows the energy spectrum plotted against \( \theta \), which is related to \( \alpha \) by the formula \( \alpha = \tan \theta \). As shown in the figure, a butterfly-like structure appears.
While the wave functions are spread over the oblique potential
in the energy spectrum plot. This structure is similar to the “3D butterfly” which is introduced in Refs. 5 and 6. We will show the reason for this similarity later. The color in Fig. 4 represents the inverse participation ratio (IPR) in each eigenfunction. Small IPR denotes that the eigenfunction is well localized. We can see that eigenstates in the band gap is well localized. These states correspond to edge states in topological systems.

C. Obliquely introduced superlattice

Now, we consider the case when $V(x)$ is periodic, in particular, we take $V_{m,n} = V cos(\phi x m + \phi y n - \delta)$. In this case, when we vary $\delta$ slowly, the Hamiltonian will be periodic in time, and this setup corresponds to the adiabatic transport, which is first proposed by D. J. Thouless[18]. It is known that the mapping between a 1D superlattice system and a 2D Hofstadter model exists. Analogously, we can clearly understand the topological aspects of our model by mapping it onto a 3D Hamiltonian. For simplicity, we start our discussion in the case of cosine type potential such as $V(x) = cos(2\pi x / L_x)$, $\alpha = L_y / L_x$, where $L_x$ and $L_y$ determine the size of the system, and we use the periodic boundary condition. Also, we use $\phi = \delta / L_x$ for the parameter of the potential shift. The Hamiltonian is written as follows:

$$\mathcal{H}(\phi) = t \sum_{m,n} \left[ \hat{c}_{m+1,n}^\dagger(\phi) \hat{c}_{m,n}(\phi) + \hat{c}_{m,n+1}(\phi) \hat{c}_{m,n}(\phi) + \text{H.c.} \right]$$

$$+ V \sum_{m,n} \cos \left( 2\pi \left( \frac{m}{L_x} + \frac{n}{L_y} \right) + \phi \right) \hat{c}_{m,n}^\dagger(\phi) \hat{c}_{m,n}(\phi).$$

(3)

We can map this Hamiltonian to a 3D Hamiltonian by using Fourier transformation,

$$\hat{c}_{m,n}(\phi) = \frac{1}{\sqrt{2\pi L_z}} \sum_{l} e^{-i\frac{\pi}{L_z} \phi} \hat{c}_{m,n,l}$$

(4)

$$\hat{c}_{m,n,l} = \frac{1}{\sqrt{2\pi L_z}} \sum_{l} e^{i\frac{\pi}{L_z} \phi} \hat{c}_{m,n}(\phi).$$

(5)

Hamiltonian (3) will be

$$\mathcal{H} = t \sum_{m,n,l} \left[ \hat{c}_{m+1,n,l}^\dagger \hat{c}_{m,n,l} + \hat{c}_{m,n+1,l}^\dagger \hat{c}_{m,n,l} + \text{H.c.} \right]$$

$$+ \frac{V}{2} \sum_{m,n,l} \left[ e^{i(2\pi \left( \frac{m}{L_x} + \frac{n}{L_y} \right) + \phi)} \right] \hat{c}_{m,n,l+1}^\dagger \hat{c}_{m,n,l} + \text{H.c.} \right].$$

(6)

This Hamiltonian implies the 3D tight-binding model on cubic lattice with a homogeneous magnetic field, whose direction is perpendicular to the $z$-axis but oblique in $xy$-plane. There are previous studies for this model, and it is known that the Hofstadter butterfly and the integer quantum Hall effect (IQHE) also appear in the 3D lattice. According to Refs. 5 and 6, each gap in the 3D Hofstadter butterfly is characterized by two Chern indices. In the 3D model, these indices are proportional to Hall conductivity. When we go back to our 2D model, these indices determine the quantum pump just like Thouless pump, and the bulk-edge correspondence shows that the quantum pump and the number of edge states match each other. In this model, quantum pump in $x$-direction and $y$-direction corresponds to the number of edge-localized states in edges of $x$-direction and $y$-direction, respectively. Also, by comparing (3) and (6), we can see that potential strength $V$ corresponds to the hopping strength in the $z$-direction. These correspondences explain why 3D butterfly appears in Fig. 4.

Here, we have only considered a cosine-type potential, but a similar mapping is also possible for other types of potentials for which there are higher frequency components, and these components will be mapped into longer distance hopping in the $z$-direction.
III. CONTINUUM MODEL OF 2D THOULESS PUMPING

A. Model

By considering the analogy of Thouless pumping and IQHE, the results in the previous section suggest that the amount of transport, as the Hamiltonian parameter \( \phi \) changes its value from 0 to \( 2\pi \), is quantized and can be expressed by the Chern number. Since the discussion in the previous section is based on the tight-binding model, it is desirable to extend our discussion to continuum systems so as to apply the results to cold atom systems. To treat the system more precisely and to see the feasibility of the previous model in the experimental setups, let us consider next a 2D continuum model.

To treat the continuum model, we consider the following Hamiltonian,

\[
H = \int dx dy \psi^\dagger(x, y) \left[ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} - \frac{\hbar^2}{2m} \frac{\partial^2}{\partial y^2} \right] \psi(x, y),
\]

\[+ V_x(x, y) + V_y(x, y) + V_{\text{SL}}(x, y) \]

where \( \psi(x, y) \) is the field operator of a particle, \( \hbar \) is Planck’s constant, and \( m \) is the mass of a particle. There are three types of potential in this system: \( V_x, V_y, \) and \( V_{\text{SL}} \). \( V_x \) and \( V_y \) form the 2D square lattice, and \( V_{\text{SL}} \) form the superlattice which is introduced obliquely to the square lattice. Now we consider two limits: one is in the limit of weak superlattice (which is called the Hofstadter regime), and the other is in the limit of strong superlattice (which is called the sliding regime).

B. Hofstadter Regime

First, we consider the regime which is near the tight-binding limit, i.e. \( V_x, V_y \ll V_{\text{SL}}/4E_L \). As we have mentioned above, in this limit, we can map our model onto a 3D cubic lattice model with an obliquely introduced homogeneous magnetic field in Eq. 6, and the amount of adiabatic pumping in our model corresponds to the quantized Hall conductivity in the cubic lattice model. In Eq. 6, \( y \) and \( z \) are cyclic coordinates, so that the wave function can be written as \( \Psi_{lmn} = e^{ik_xl + ik_ym} F_l \), where \( k_x \) and \( k_y \) are the Bloch wave numbers along the \( x \) and \( y \) directions. Then the Schrödinger equation will be

\[
t(F_{l-1} + F_{l+1})
- V \{ \cos(2\pi l/L_x + k_x) + \cos(2\pi l/L_y + k_y) \} F_l = EF_l.
\]

FIG. 5. Time evolution of the average of center of mass for the 10 lowest energy states in the case of (a) \( p_x/q_x = 2/3, p_y/q_y = 2/5 \) and (b) \( p_x/q_x = 1/3, p_y/q_y = 1/4 \).

FIG. 6. Time evolution of the average of center of mass for the 10 lowest energy states in the case of (a) \( v_{\text{SL}} = 0.5 \), (b) \( v_{\text{SL}} = 5.0 \).
phantine equation can be shown \[4\],
\[
\frac{r}{Q} = s + t_x \frac{p_x}{q_x} + t_y \frac{p_y}{q_y}.
\]
(12)

Here, \( r \) is the number of filled bands and \( Q \) is the least common multiple of \( q_x \) and \( q_y \). \( t_x \) and \( t_y \) correspond to the amount of the charge transport while \( \varphi \) changes from 0 to \( \pi/Q \). The details of the proof of this equation is noted in Appendix.

Figure 5 shows concrete examples of such quantized pumping. Figures 5 (a) and (b) are the time evolution of the center of mass for the 10 lowest energy states in the case of (a) \( p_x/q_x = 2/3, p_y/q_y = 2/5 \) and (b) \( p_x/q_x = 1/3, p_y/q_y = 1/4 \), respectively. According to Fig. 5, particles are pumped in the \( y = x \) direction for (a), and the \( y = -x \) direction for (b). Surprisingly, while the direction of the superlattice is changed only slightly, the pumping direction is completely changed. This pumping direction can be predicted by solving Eq. (12) with the condition \( r = 1 \) since the lowest band contribution is dominant. For example, in the case (a), the solution of Eq. (12) is \( (t_x, t_y) = (1 + 3m, 1 + 5n) \). \( t_x \) and \( t_y \) correspond to the order of perturbation. Therefore, although there are an infinite number of solutions, only the solution where \( |t_x| \) and \( |t_y| \) have the smallest values is dominant. In the case (a), that is \( t_x, t_y = (1, 1) \).

Similarly, in the case (b), the solution of the Diophantine equation is \( (t_x, t_y) = (1 + 3m, -1 + 4n) \), however, the dominant solution is \( (t_x, t_y) = (1, -1) \). These results are consistent with Fig. 5.

Observing Fig. 5 carefully, we find a small oscillations after the particle was pumped to the next lattice. This oscillation occurs at the moment when the ground state energies in two sites become close. At that moment, the potential shape can be approximated by a double well, and the particles oscillate between the double well. Since the angular frequency of this oscillation will be the same as the hopping amplitude \( J \), the period will be \( T = 2\pi/J \). To estimate \( J \) in the optical lattice, we can use \( J = \frac{\sqrt{2}}{3} \sqrt{s} \exp(-2\sqrt{s}) \) where \( s = V_L/E_R \) \[40\].

We have checked that this estimate is consistent with the numerical result in Fig. 5. We have also verified that the frequency of this small oscillation does not change while we change the time period \( T \). This result implies that the small oscillation is caused by the pumping which is performed in finite time. Therefore, we expect that this small oscillation disappears in the adiabatic limit.

C. Sliding Regime

In the opposite limit, where the \( V_{SL} \) term is dominant, the pumping behavior changes completely. From our numerical simulation, we find that the pumping direction is restricted to the \( x \)-axis or the \( y \)-axis exactly in this limit. More precisely, the pumping direction will be whichever is closer to the \( x \)-axis or the \( y \)-axis.

When \( V_{SL} \) varies across the Hofstadter regime to the sliding regime, the topological transition occurs. Figures 6 and 7 provide concrete examples of such topological transition. Figures 6 (a) and (b) show the time evolution of the center of mass for the 10 lowest energy states in the case of \( p_x/q_x = 2/3, p_y/q_y = 1 \), with (a) \( v_{SL} = 0.5 \) and (b) \( v_{SL} = 5 \). (a) is an example of those in the Hofstadter regime and (b) in the sliding regime. In (a), particle moves towards negative \( x \) direction. On the contrary, in (b), it moves towards positive \( x \) direction.

FIG. 7. Particle density profiles for the 10 lowest energy states in the case of \( p_x/q_x = 2/3, p_y/q_y = 1 \), with (a) \( v_{SL} = 0.5 \) and (b) \( v_{SL} = 5 \).

(a) is an example of those in the Hofstadter regime and (b) in the sliding regime. In (a), particle moves towards negative \( x \) direction. On the contrary, in (b), it moves towards positive \( x \) direction. Figure 6 shows concrete examples of such quantized pumping. Figures 6 (a) and (b) are the time evolution of the center of mass for the 10 lowest energy states in the case of (a) \( p_x/q_x = 2/3, p_y/q_y = 2/5 \) and (b) \( p_x/q_x = 1/3, p_y/q_y = 1/4 \), respectively. According to Fig. 6, particles are pumped in the \( y = x \) direction for (a), and the \( y = -x \) direction for (b). Surprisingly, while the direction of the superlattice is changed only slightly, the pumping direction is completely changed. This pumping direction can be predicted by solving Eq. (12) with the condition \( r = 1 \) since the lowest band contribution is dominant. For example, in the case (a), the solution of Eq. (12) is \( (t_x, t_y) = (1 + 3m, 1 + 5n) \). \( t_x \) and \( t_y \) correspond to the order of perturbation. Therefore, although there are an infinite number of solutions, only the solution where \( |t_x| \) and \( |t_y| \) have the smallest values is dominant. In the case (a), that is \( t_x, t_y = (1, 1) \).

Similarly, in the case (b), the solution of the Diophantine equation is \( (t_x, t_y) = (1 + 3m, -1 + 4n) \), however, the dominant solution is \( (t_x, t_y) = (1, -1) \). These results are consistent with Fig. 5.

Observing Fig. 5 carefully, we find a small oscillations after the particle was pumped to the next lattice. This oscillation occurs at the moment when the ground state energies in two sites become close. At that moment, the potential shape can be approximated by a double well, and the particles oscillate between the double well. Since the angular frequency of this oscillation will be the same as the hopping amplitude \( J \), the period will be \( T = 2\pi/J \). To estimate \( J \) in the optical lattice, we can use \( J = \frac{\sqrt{2}}{3} \sqrt{s} \exp(-2\sqrt{s}) \) where \( s = V_L/E_R \) \[40\]. We have checked that this estimate is consistent with the numerical result in Fig. 5. We have also verified that the frequency of this small oscillation does not change while we change the time period \( T \). This result implies that the small oscillation is caused by the pumping which is performed in finite time. Therefore, we expect that this small oscillation disappears in the adiabatic limit.
approximated by eigenstates in the harmonic potential, and the
eigenenergies are expressed as $E = \hbar \omega (n + 1/2)$. The
transition occurs when the energy difference between the
ground state and the first excited state is close to $2v_{SL}$.
Since the transition point is $v_{SL} \sim \sqrt{\frac{\pi^2 v_{SL}}{md^2}}$, in Fig. 6 and
Fig. 7, we have chosen $v_L = 1.0, \frac{\pi^2}{md^2} = \frac{\pi^2}{3}$; therefore, the
transition point is estimated to be $v_{SL} = \frac{\pi}{2} = 1.57 \ldots$
This is consistent with Fig. 6 and Fig. 7.

IV. CONCLUSION

We have proposed a 2D version of Thouless pumping
which can be realized by using ultracold atoms in an
optical lattice. We considered a 2D square lattice tight-
binding model with an obliquely introduced superlattice.
We showed that quantized particle transport occurs in
this system, and the transport is expressed as a solu-
tion of the Diophantine equation. This topological nature
could be understood easily by mapping the hamiltonian
onto a 3D cubic lattice model with a homogeneous mag-
netic field. On the other hand, in the weak potential
limit, we have uncovered that the amount of the quan-
tized transport is restricted to exactly $x$-axis or $y$-axis
direction. This difference in two limits causes a topo-
logical transition. Furthermore, we have demonstrated
by numerical simulations that the above phenomena are measurable in a cold atom system.

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Appendix A: Derivation of Diophantine equation in
tight-binding limit

In this Appendix, we derive Eq. 12 from the Hamilton-
ian,

$$H(\phi) = t_x \sum_{m,n} \left[ \hat{c}_m^{\dagger} \hat{c}_{m+1,n}(\phi) + \text{h.c.} \right]$$

$$t_y \sum_{m,n} \left[ \hat{c}_m^{\dagger} \hat{c}_{m,n+1}(\phi) + \text{h.c.} \right]$$

$$+ V \sum_{m,n} \cos \left( 2\pi (\Phi_x m + \Phi_y n) + \phi \right) \hat{c}_m^{\dagger} \hat{c}_{m,n}(\phi)$$

(A1)

This Hamiltonian is periodic in $\phi$ with period $2\pi$. Here, we
suppose that $\Phi_x, \Phi_y$ are rational numbers, such as
$\Phi_x = p_x/q_x, \Phi_y = p_y/q_y$.

The Fourier-transformed Hamiltonian is

$$H = -\int_{-\pi}^{\pi} \frac{dk_x}{2\pi} \int_{-\pi}^{\pi} \frac{dk_y}{2\pi} \left[ t \left( \cos(k_x) + \cos(k_y) \right) \hat{c}_m^{\dagger}(k_x,k_y,k_z) \hat{c}(k_x,k_y,k_z) 
\right.

+ \frac{V}{2} \left( e^{-ik_x} \hat{c}_m^{\dagger}(k_x + 2\pi\Phi_x,k_y + 2\pi\Phi_y,k_z) \hat{c}(k_x,k_y,k_z)
\right.

+ e^{ik_x} \hat{c}_m^{\dagger}(k_x - 2\pi\Phi_x,k_y - 2\pi\Phi_y,k_z) \hat{c}(k_x,k_y,k_z) \right] .$$

(A2)

Here, we define $k_z = 2\pi/p_z$ for convenience. However, there
is a mixing between $(k_x, k_y, k_z) \rightarrow (k_x \pm 2\pi\Phi_x, k_y \pm 2\pi\Phi_y, k_z)$ and thus the Hamiltonian is not diagonal in
$k$. To diagonalize this, we need to separate $k_x, k_y$ into
$q_x \times q_y$ regions as follows,

$$k_x = k_x^0 + 2\pi\Phi_x m$$

$$k_y = k_y^0 + 2\pi\Phi_y n .$$

(A3)

(A4)

Then, the Hamiltonian can be written as:

$$H = \frac{1}{(2\pi)^3} \int_{-\pi/q_x}^{\pi/q_x} dk_x^0 \int_{-\pi/q_y}^{\pi/q_y} dk_y^0 \int_{-\pi}^{\pi} dk_z \hat{H}(k_x^0, k_y^0, k_z)$$

(A5)

Note that the Brillouin zone is reduced to $[-\pi/q_x, \pi/q_x]$ for $k_x$ and $[-\pi/q_y, \pi/q_y]$ for $k_y$. Now, the Schrödinger
equation $\hat{H}(k_x^0, k_y^0) \ket{\psi} = E_{k_x^0, k_y^0} \ket{\psi}$ is reduced to that for a 1D tight-binding model. The single particle energy is obtained by expanding the state into single-particle states at each lattice point $m$,

$$|\psi\rangle = \sum_{m=0}^{q-1} a_m e^{i k_x^0 m + 2\pi \Phi_x m, k_y^0 + 2\pi \Phi_y m, k_z^0} |0\rangle \quad (A7)$$

where $|0\rangle$ is the vacuum. The eigenvalue equation is

$$(-2t \cos (k_x^0 + 2\pi \Phi_x n) - 2t \cos (k_y^0 + 2\pi \Phi_y n)) a_n - \frac{V}{2} (e^{-ik_x a_{n-1}} + e^{ik_x a_{n+1}}) = E_{k_x^0, k_y^0, k_z^0} a_n. \quad (A8)$$

This corresponds to the Harper equation for the Hofstadter model. Let $Q$ be the least common multiple of $q_x$ and $q_y$. For convenience, we perform the transformation

$$a_j = \sum_{l=0}^{Q-1} e^{i 2\pi j l/Q} b_l \quad (A9)$$

and we obtain

$$-t_x (e^{ik_x b_{j+p_x}} + e^{-ik_x b_{j-p_x}})$$
$$-t_y (e^{ik_y b_{j+p_y}} + e^{-ik_y b_{j-p_y}}) \quad (A10)$$
$$-V \cos \left(k_z + \frac{2\pi j}{Q}\right) b_j = E_{k_x^0, k_y^0, k_z^0} b_j.$$

To solve this equation, we apply the perturbation theory under the condition $t_x, t_y \ll V$. The solution at $t_x, t_y = 0$ is

$$E_m (k_x^0, k_y^0, k_z^0) = -2t_a \cos \left(k_z + \frac{2\pi m}{Q}\right), \quad \psi_j = \delta_{j,m}. \quad (A11)$$

If we make $t_x, t_y$ finite, gaps open at the degeneracy points. To understand the details, we should make the condition for degeneracy clear. When the two bands $\psi_{m_1}$ and $\psi_{m_2}$ cross each other, the degeneracy condition is

$$k_z + \frac{2\pi}{Q} m_1 = -\left(k_z + \frac{2\pi}{Q} m_2\right) \pmod{2\pi}. \quad (A12)$$

The degeneracy only occurs when $k_z = 0, \pm \pi/q$, so we can rewrite it as

$$m_1 + m_2 + l \equiv 0 \pmod{q} \quad (l \in \{0, \pm 1\}, l = qk_z^0/\pi). \quad (A13)$$

It is obvious that the lowest band is $m_0 = 0$. It is possible to determine all of the band indices by using Eq. A13. There is a simple relation between the gap number $r$ and band indices $m_1, m_2$,

$$r \equiv -|m_1 - m_2| \pmod{Q}. \quad (A14)$$

Now we are ready to use the perturbation theory. Since the $t_x(t_y)$ term only mixes two sites which are $P_x(P_y)$ sites apart from each other, in order to hybridize $\phi_{m_1}$ and $\phi_{m_2}$, the following equation must be satisfied,

$$|m_1 - m_2| = P_x t_r + P_y u_r \pmod{Q} \quad (A15)$$

that is,

$$r/Q = s_r + p_x/q t_r + p_y/q u_r. \quad (A16)$$

The lowest order of perturbation which mixes $\phi_{m_1}$ and $\phi_{m_2}$ is the $|t_r|$th order for $t_x$ term, and $|u_r|$th order for the $t_y$ term, respectively.

The Hamiltonian around the $r$th gap is

$$\left(\begin{array}{c}
\epsilon e^{ik_x t_x} e^{ik_y u_y} \\
\Delta e^{-ik_x t_x} e^{-ik_y u_y} - \epsilon
\end{array}\right) \left(\begin{array}{c}
a \\
b
\end{array}\right) = E \left(\begin{array}{c}
a \\
b
\end{array}\right) \quad (A17)$$

Now, it is possible to calculate the amount of pumping in one cycle from this Hamiltonian. The pumping amount will be $t_r$ for $x$-direction and $u_r$ for $y$-direction, and this is exactly the solution of Diophantine equation (A16). However, we should be aware that “one cycle” here corresponds to the width of Brillouin zone of $k_z$, while $k_z$ changes its value $2\pi/Q$.

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