Diffusion Suppressed Topological Thouless Pumping

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In Thouless pumping, although non-flat band has no effects on the quantization of particle transport, but it induces wave-packet diffusion which hinders the practical applications of Thouless pumping. Indeed, we find that the diffusion mainly arises from the dynamical phase difference between individual Bloch states. Here we propose two efficient schemes to suppress diffusion in Thouless pumping: (i) the re-localization echo protocol and (ii) the high-order tunneling suppression protocol. In the first protocol, we reverse the Hamiltonian in the second pumping cycle to cancel the dynamical phase difference arise from non-flat band and re-localize the diffused wave-packet. In the high-order tunneling suppression protocol, we modulate the nearest neighbor tunneling strength to suppress the high-order tunnelings which cause wave-packet diffusion. At the same time, we find that the applied modulation makes the Bloch band more flat. Our study paves a way toward the diffusionless Thouless pumping for practical applications in matter transport, state transfer, and quantum communications.

Introduction. Topological Thouless pumping \cite{1}, a quantized transport in a one-dimensional cyclically modulated periodic potential, has attracted a great attention. In addition to the electronic systems \cite{1}, several other systems, such as ultracold atomic systems \cite{2} and photonic waveguide arrays \cite{3}, have been proposed to implement the Thouless pumping. Moreover, the Thouless pumping have been generalized to interacting systems \cite{3, 4, 6}, high dimensional systems \cite{7}, and energy pumping in Floquet systems \cite{8–10}.

The implementation of Thouless pumping has to satisfy two key conditions: (i) the system undergoes adiabatic evolution, and (ii) the initial state uniformly fills the evolved Bloch band. It has been demonstrated that the Thouless pumping is not robust against non-adiabatic effects and the realistic transport deviates from the ideally quantized transport described by the topological Chern number \cite{11–13}. Generally, the initial state can be chosen as the Wannier state which equally populates the evolved Bloch band. The more flat the Bloch band is, the more localized the Wannier state is. In one pumping cycle, the position shift of the input Wannier state directly relates to the Chern number of the filled band \cite{14, 15}. In recent experiments, the Thouless pumping have been successfully implemented via cold atoms in modulated optical lattices \cite{16, 17}. However, it is a great challenge to maintain perfectly flat bands during the whole pumping process. A natural question arises: How does a non-flat band affect the Thouless pumping?

In one adiabatic pumping cycle, the system will acquire both Berry phase and dynamical phase. The accumulated phases make a gauge transformation of the input Wannier state and affect the spatial distribution of the output state \cite{3}. Although a non-flat band does not affect the quantized position shift, it makes a major contribution to the wave-packet diffusion even under adiabatic evolution. The diffusion delocalizes the input Wannier state. Therefore large-size systems are needed to avoid the boundary effects and more times of position measurement are needed to determine the Chern number. Moreover, the diffusion will hinder the practical applications of Thouless pumping in matter transport, state transfer, and quantum communication \cite{18–20}.

In this Letter, we propose two protocols to suppress the diffusion during the Thouless pumping: (i) the re-localization echo protocol and (ii) the high-order tunneling suppression protocol. In the first protocol, the Hamiltonian $\hat{H}(t)$ in the first pumping cycle is changed to $-\hat{H}(t)$ in the second pumping cycle. The diffused wave-packet in the first cycle becomes re-localized in the second cycle. The key feature of this protocol is that the dynamical phases of individual Bloch states during the two cycles have opposite signs but with the same magnitude and thus the final dynamical phases after every two cycles vanish. In the second protocol, due to the diffusion in the Thouless pumping mainly attributes to some high-order tunnelings, we propose to modulate the nearest neighbour tunneling strength to switch off the high-order tunnelings and then suppress the diffusion. Actually, the successful diffusion suppression attributes to that the modulation makes the Bloch band more flat.

Model. We consider the generalized one-dimensional commensurate Aubry-André-Harper (AAH) model \cite{21, 22} described by the following tight-binding Hamiltonian

$$\hat{H}(t) = \sum_j \left( J_j(t)c_j^\dagger c_{j+1} + \text{H.c.} \right) + \sum_j V_j(t)c_j^\dagger c_j. \quad (1)$$

We assume it has $L$ cells and each cell consists of $q$ sites.
Thus the total sites is $N = qL$. Here $c_j^\dagger$ and $c_j$ are respectively creation and annihilation operators for the $j$-th site. For simplicity, we alternately denote the sites $3l - 2$, $3l - 1$, and $3l$ as $A$, $B$, and $C$, and their corresponding potentials as $V_A$, $V_B$, and $V_C$, see Fig. 2. $J_j(t)$ and $V_j(t) = V_0 \cos(2\pi \beta j + \phi(t))$ are respectively the nearest-neighbouring tunneling strength and the on-site potential. $J_j(t) = -J$ for the re-localization echo protocol and $J_j(t) = -J \sin(2\pi \beta j + \phi(t))$ for the higher-order tunneling suppression protocol. $V_0$ describes the diagonal modulation amplitude and the rational parameter $p/q$ (in our calculation, we choose $\beta = p/q$) determines the modulation frequency. In our calculation, we choose $\beta = p/q = 1/3$ for both protocols, the time-dependent modulation phase $\phi(t)$ is adiabatically swept according to $\phi(t) = \omega t + \phi_0$ with the ramping speed $\omega$ and the initial modulation phase $\phi_0$ and the pumping period $T = 2\pi/\omega$. 

Similar to other Thouless pumping systems [23], our system is periodic both in space and time. We can use the Chern number $C_m$ to characterize the topological features of its pumping process. It is defined as

$$ C_m = \frac{1}{2\pi} \int_{-\pi/q}^{\pi/q} dk \int_0^T dt F_m(k, t), \quad (2) $$

on the Brillouin-like zone $(-\pi/q < k < \pi/q, 0 < t \leq T)$. Here $F_m(k, t) = i\langle \partial_t u_m | \partial_k u_m - \partial_k u_m | \partial_t u_m \rangle$ is the Berry curvature and $|u_m(k, t)\rangle$ is the periodic part of the Bloch state $|\psi_m(k)\rangle$. 

In the Thouless pumping, the initial state can be chosen as Wannier state [24]

$$ |W_m(R)\rangle = \frac{1}{\sqrt{L}} \sum_k e^{-ikR} |\psi_m(k)\rangle, \quad (3) $$

where $R$ is the cell index of the Wannier state and $m$ denotes the Bloch band index. Due to the freedom in choosing the phase of Bloch states, $e^{i\theta(k)}|\psi_m(k)\rangle$, the Wannier states are arbitrary. Fortunately, by minimizing the spread function, $\Omega = \langle X^2 \rangle - \langle X \rangle^2$, one can get the unique maximally localized Wannier states (MLWSs) [1–3]. In which, the position operator is defined as $\hat{X} = \sum_{j=1}^{qL} j \hat{n}_j$ with $\hat{n}_j = c_j^\dagger c_j$. In a pumping cycle, $\phi(t)$ changes adiabatically by $2\pi$ and the mean position shift of the Wannier state is given as

$$ \Delta P = qC_m. \quad (4) $$

This relationship depends only on the band topology and it is independent of the evolution details. However, the non-flat band makes difference on the dynamical phases of individual Bloch states and this difference makes the input MLWS diffused. The wave-packet diffusion can be characterized by the diffusion width $D_W = \sqrt{\Omega}$, which is the square root of the spread function $\Omega$. During the pumping process, the spread function can be decomposed as two terms $\Omega = \Omega_I + \Omega_D$ [1, 3]. The gauge invariant term $\Omega_I$ does not change during the whole pumping procedure and the time-varying term $\Omega_D$ is zero for the initial MLWSs. Therefore the diffusion after one pumping cycle is determined by

$$ \Omega_D(T) = \frac{q}{2\pi} \int_{-\pi/q}^{\pi/q} \left( X_d(k) + X_b(k) - qC_m \right)^2 dk, \quad (5) $$

with the displacements $X_d(k) = -\frac{\partial}{\partial k} \gamma_d(k)$ and $X_b(k) = -\frac{\partial}{\partial l} \gamma_b(k)$ of a Bloch state with quasi-momentum $k$ (here and hereafter we set $\hbar = 1$). Here $\gamma_d(k) = -\int_0^T E_m(k, t) dt$ is the dynamical phase and $\gamma_b(k) = i \int_0^T \langle u_m | \partial_t u_m \rangle dt$ denotes the Berry phase. Actually, the quantized transport $qC_m$ is just the average value of $X_b(k)$ over the Brillouin-like zone. The term $X_d(k)$ arises from the dynamical phase difference caused by the non-flat band. The phase difference accumulated in the pumping process makes a major contribution to the diffusion, and so that more significant wave-packet diffusion appears for more slow modulation. In contrast, the other term $\Omega_d(k)$ does not depend on the evolution time. Under strongly diagonal modulations (i.e. $|J/V_0| \ll 1$), the term $X_d(k)$ is the main source of diffusion in the adiabatic Thouless pumping (see more details in the Supplementary Material [27]).

Re-localization echo protocol. In this protocol, we discuss how to suppress the diffusion via cancelling the dynamical phases. The system evolves under $\hat{H}(t)$ in the first cycle and then $-\hat{H}(t)$ in the second cycle. At begin, each individual Bloch state $|\psi_m(k, 0)\rangle$ has no dynamical phase, see the horizontal arrows in Fig. 1 (e). The dynamical phase difference increase with the evolution time during the first cycle, the anticlockwise-rotating arrows with different frequencies. In the second cycle, since the Hamiltonian changes from $\hat{H}(t)$ to $-\hat{H}(t)$, the eigenstate index changes from $m$ in the first cycle to $m' = q + 1 - m$ in the second cycle, and the energy bands become reversed, see the insets in Fig. 1 (e). This means that the corresponding Wannier state also changes from the $m$-th band of $\hat{H}(t)$ to the $m'$-th band of $-\hat{H}(t)$. As $|\psi_m(k, t)\rangle$ and $|\psi_{m'}(k, T + t)\rangle$ represent the same quantum state, this ensures that the Berry phases accumulated in the two cycles are equal. Thus the Chern numbers for the two bands are exactly the same. Since the mean position shift $\Delta P$ only depends on the Chern number, it takes the same value in each cycle. 

Due to the band inversion, the Bloch states $|\psi_m(k, t)\rangle$ and $|\psi_{m'}(k, T + t)\rangle$ evolve with opposite energy. As a result, the dynamical phase for the second cycle $\gamma_d^{(2)}$ is just the opposite to the one for the first cycle $\gamma_d^{(1)}$, that is, $\gamma_d^{(2)} = \frac{\partial}{\partial k} \langle \psi_m(k, t) | \hat{H}(t) | \psi_{m'}(k, t) \rangle dt = -\int_0^T \langle \psi_m(k, t) | \hat{H}(t) | \psi_{m'}(k, t) \rangle dt = -\gamma_d^{(1)}$. Consequently, the dynamical phases accumulated in the second cycle cancel the ones accumulated in the first cycle, see the clockwise-rotating arrows back to the initial direction in Fig. 1 (e). The blue solid (dashed) lines respectively...
denote the dynamical phases of the Bloch states corresponding to the solid (dashed) circles in the bands. In contrast, in the traditional Thouless pumping without reversing the sign of $H(t)$, the dynamical phase difference and the diffusion width will increase with the evolution time [see Fig. 1 (f)].

![Figure 1](image_url)

FIG. 1. (color online). Thouless pumping during two pumping cycles: (i) the re-localization echo protocol (left column), and (ii) the traditional protocol (right column). (a) and (b): the density distribution $n_j$ versus the time $t/T$. (c) and (d): the mean position shift $\Delta P$ (blue solid line) and the diffusion width $D_W$ (red dashed line) versus the time $t/T$. (e) and (f): the dynamical phase $\gamma_d(k)$ versus the time $t/T$. The insets in (e) and (f) illustrate the energy bands. The black dashed arrows and blue dashed line correspond to the red point in dashed circle. The black solid arrows and blue solid line correspond to the point in solid circle present. The parameters are chosen as $N = 45$, $J = 1$, $V_0 = 30$, $\phi_0 = 0$ and $\omega = 0.01$.

In Fig. 1, we compare our re-localization echo protocol with the traditional Thouless pumping. At begin, the particle stays in the 27-th site (i.e. the C-sublattice at the 9-th cell), which is labeled as $|C\rangle_9$. The initial state has 99.9% projection on the MLWS for the highest band. In the first cycle, the density distribution gradually spreads with the evolution time. In the second cycle, for the traditional Thouless pumping, the density distribution spreads as the one in the first cycle, see Fig. 1 (b). However, for our re-localization echo protocol, the density distribution re-localizes in the second cycle and the final distribution almost evolves back to its initial shape, see Fig. 1 (a). The final state for our re-localization echo protocol has 98.9% projection on the MLWS $|C\rangle_7$, but the one for the traditional Thouless pumping has only a very small amount on $|C\rangle_7$. Although the mean position shifts $\Delta P$ are almost the same (2 unit cells) for both our re-localization echo protocol [see Fig. 1 (c)] and the traditional Thouless pumping [see Fig. 1 (d)], the corresponding diffusion widths are very different. In our re-localization echo protocol, the diffusion width $D_W$ (red dashed line) gradually increases in the first cycle and then gradually decrease to 0 in the second cycle, see Fig. 1 (c). In the traditional Thouless pumping, the diffusion width $D_W$ (red dashed line) keeps increase with the evolution time, see Fig. 1 (d). Thus, although the mean position shifts are both determined by Chern number, the wave-packet diffusion are strongly suppressed by our re-localization echo protocol.

**High-order tunneling suppression protocol.** The diffusion mechanism in the Thouless pumping can also attribute to the high-order quantum tunneling. Under strongly diagonal modulations ($|J/V_0| \ll 1$), due to the first-order resonant tunneling, the mean position shift mainly occurs around the time when the on-site potentials of neighboring sites are equal [see Fig. 1]. If the particle only jumps to the nearest neighbouring site and the wave-packet will keep localized. However, at the same time, the high-order resonant tunneling also takes place and thus the wave-packet diffuses [as shown in Fig. 2 (c)]. As a result, the diffusion width $D_W$ grows drastically around the resonant points [see Fig. 1]. Unlike the first-order resonant tunneling, which is unidirectional, the high-order resonant tunneling always occurs between neighbouring cells and has equal probability toward the two opposite directions.

To describe the diffusion caused by the inter-cell tunneling, we derive the effective model via applying degenerate perturbation theory up to the third-order [4, 5]. Under strongly diagonal modulations ($|J/V_0| \ll 1$), we treat the tunneling term $\tilde{V} = \sum_{j=1}^{N-1} (J_j c_j^\dagger c_{j+1} + \text{H.c.})$, as a perturbation to the on-site energy term $\tilde{H}_0 = \sum_{j=1}^{N} V_j c_j^\dagger c_j$. Since different resonant points corresponding to different effective Hamiltonians, we decompose one pumping cycle as three regions: (I) around the first resonant point where $V_A = V_B$, (II) around the second resonant point where $V_B = V_C$, and (III) around the third resonant point where $V_C = V_A$. In the Supplementary Material [27], we give the details for deriving the effective Hamiltonians.

To understand the diffusion process, we discuss how the inter-cell high-order resonant tunnelings appear. As an example, we consider the system evolves from the state of the particle in the 27-th site (i.e. the sublattice $C$ of the 9-th cell). That is, the system evolves from the region (I). Because of the large potential bias, it will stay in the sublattice $C$ until the tunneling strength is comparable to the potential bias. The three-order resonant tunneling makes the particle move to corresponding sublattices in adjacent cells, that is, from sublattice $C$ in $l$-th cell to sublattice $C$ in $(l-1)$-th and $(l+1)$-th cells, see Fig. 2 (c1). Since the leftward and rightward three-order tunnelings have the same strength, they do not change the mean position shift and may only cause wave-packet diffusion. Then, according to the on-site modulation $V_j(t) = V_0 \cos(2\pi J_j + \phi(t))$,
the system evolves into the region (II). In the vicinity of $V_B = V_c$, due to the effective first-order tunneling $j_{II}^{(1)}(\langle B|\langle C| + H.c.)$, the particle jumps from the sublattice $C$ to its nearest neighboring sublattice $B$. Here $j_{II}^{(1)} = J_2 - J_2(\hat{J}_2^2 + \hat{J}_3^2)/(2\Delta_1\Delta_3)$ with $\Delta_1 = V_A - V_B$, $\Delta_2 = V_B - V_c$ and $\Delta_3 = V_A - V_c$. The second term in $j_{II}^{(1)}$ represents a correction term from the third-order processes. In addition to the first-order resonant tunneling $|C\rangle\rightarrow |B\rangle$, the second-order resonant tunnelings $|C\rangle\rightarrow |B\rangle_{l+1}$ and $|B\rangle\rightarrow |C\rangle_{l+1}$ may occur at the same time, which are described by $J_{II}^{(2)}(\langle B|\langle C| + H.c.)$ with $J_{II}^{(2)} = -J_1J_3(1/\Delta_1 + 1/\Delta_3)/2$. In particular, the wave-packet diffusion becomes significant due to these second-order tunnelings connect with the first-order ones, that is, $|C\rangle_{l+1} \rightarrow |B\rangle_{l+1} \rightarrow |C\rangle_{l+1}$ and $|C\rangle_{l+1} \rightarrow |B\rangle_{l} \rightarrow |C\rangle_{l+1}$ [see Fig. 2 (c2)]. In the whole process, the third-order resonant tunnelings [which are described by $j_{III}^{(3)}(\langle C|_{l+1} + H.c.)$ with $j_{III}^{(3)} = J_1J_3J_3(2\Delta_1\Delta_3)$] always take place. The time-evolution in all regions are similar: the third-order resonant tunnelings and the connected second-order-to-first-order resonant tunnelings cause wave-packet diffusion, but do not affect the mean position shift.

To suppress the wave-packet diffusion, one may switch off the high-order resonant tunnelings. In general, there are several different schemes to switch off the high-order resonant tunnelings. We find that one can switch off the high-order resonant tunnelings via modulating the tunneling strengths according to

$$J_j(t) = -J\sin(2\pi\beta j + \phi(t)).$$

Obviously, at the resonant point $V_B(t) = V_c(t)$, $\{J_1, J_2, J_3\}$ are respectively $\{0, \sqrt{3}/2, -\sqrt{3}/2\}$. Thus we have the high-order tunneling strengths $J_{III}^{(2)} = J_{III}^{(3)} = 0$. Similarly, at other resonant points [see Fig. 2 (a)], the high-order tunnelings are also switched off. Moreover, this modulation makes the Bloch band more flat (see more details in the Supplementary Material [27]).

In Fig. 2, we show the diffusion suppressed topological Thouless pumping under the hopping modulation (6). In the top panel of Fig. 2 (b), we show the time-evolution of the density distribution $\langle\hat{n}_l\rangle$. The initial state is $|C\rangle_1$ whose projection on the MLWS for the highest band is 99.9%. The density distribution is well localized during the whole pumping process and the final state has 99.9% projection on the state $|C\rangle_1$. In the bottom panel of Fig. 2 (b), we show the mean position shift $\Delta P$ (blue solid line) and the diffusion width $D_W$ (red dashed-dot line). The mean position shifts $-0.999$ unit cells, which is very close to the Chern number $-1$ for the highest band. The diffusion width $D_W$ is very small during whole process and the sharp peaks correspond to the steps in $\Delta P$. However, if the tunneling strengths are fixed, the diffusion width $D_W$ will increase with time, see the gray dashed line in the bottom panel of Fig. 2 (b).

**Summary and Discussions.** In the Thouless pumping, even under adiabatic evolutions, the non-flat bands will bring non-uniformly dynamical phases and then induce wave-packet diffusion. We have put forward two protocols to achieve diffusion suppressed Thouless pumping. In re-localization echo protocol, the initial MLWS will expand in the first cycle and it gradually localizes during the second cycle via reversing the Hamiltonian. In high-order tunneling suppression protocol, by modulating the nearest-neighbouring tunneling strengths, the wave-packet is almost diffusionless during the whole pumping process. In both protocols, the particle transports are well consistent with the quantized ones given by the Chern number and the final wave-packets almost perfectly return to their input shapes. Our studies pave a way toward implementing long-distance diffusionless Thouless pumping for practical applications.

Lastly, we briefly discuss the experimental feasibility. Due to rich manipulation techniques, such as individual site control and large range of tunable parameters, our protocols can be realized via superconducting quantum circuits [30–34]. It has been demonstrated that, through controlling the flux threading the non-hysteretic rf SQUID loop between the two resonators, the coupling strength between two superconducting transmission line resonators can be tuned from negative to positive [35]. This experimental technique enables the desired hopping modulations in our system. Moreover, one may use the

![FIG. 2. (color online). Diffusion suppressed Thouless pumping under periodic modulations. (a) Periodic modulations of the on-site energies and the nearest-neighbouring tunnelings. (b) Top: the density distribution $\langle\hat{n}_l\rangle$. Bottom: the mean position shifts $\Delta P$ and the diffusion width $D_W$. The blue solid and red dashed lines denote $\Delta P$ and $D_W$, respectively. The gray dashed line corresponds to the system with fixed tunneling strengths. (c) High-order resonant tunnelings in regions (I) and (II). The other parameters are set as the ones for Fig. 1.](image-url)
photonic lattices with complex couplings as a potential platform for testing our protocols [36].

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SUPPLEMENTARY MATERIALS

Relation between mean position shift and Chern number

At the initial time $t = 0$, the input state for performing Thouless pumping is chosen as the Wannier state

$$|W_m(R, 0)⟩ = \frac{1}{\sqrt{L}} \sum_k e^{-ikqR} |ψ_m(k, 0)⟩ = \frac{1}{\sqrt{L}} \sum_{k,j} e^{-ikqR} e^{ikj} u_{m,j}(k,0)c_j^†|0⟩,$$

(S7)

where $u_{m,j}(k,0) = u_{m,j+q}(k,0)$ is the periodic part of the Bloch function. Applying the position operator $\hat{X}$ on the Wannier state, we have

$$\hat{X}|W_m(R, 0)⟩ = \frac{1}{\sqrt{L}} \sum_{k,j} e^{-ikqR} e^{ikj} u_{m,j}(k,0)j^†c_j^†|0⟩$$

$$= qR|W_m(R, 0)⟩ + \frac{1}{\sqrt{L}} \sum_{k,j} e^{-ikqR} e^{ikj} i \frac{∂}{∂k} u_{m,j}(k,0)c_j^†|0⟩.$$

(S8)

Here we use the relation $\frac{∂}{∂k}|W_m(R, t)⟩ = 0$. Thus the mean position at $t = 0$ is given as

$$⟨\hat{X}_m(0)⟩ = qR + \frac{1}{L^2} \sum_{k,k',j} e^{-i(k-k')qR} e^{i(k-k')j} u_{m,j}^*(k',0) i \frac{∂}{∂k} u_{m,j}(k,0)$$

$$= qR + \frac{1}{L^2} \sum_{k,k'} e^{-i(k-k')qR} \sum_{R'=0}^{L-1} e^{i(k-k')(R'+j')} u_{m,j}^*(k',0) i \frac{∂}{∂k} u_{m,j}(k,0)$$

$$= qR + \frac{1}{L} \sum_k \sum_{j'=1}^{q} u_{m,j}^*(k,0) i \frac{∂}{∂k} u_{m,j}(k,0)$$

$$= qR + \frac{1}{L} \sum_k ⟨u_m(k,0)|i \frac{∂}{∂k}|u_m(k,0)⟩,$$

(S9)

where we denote

$$|u_m(k,0)⟩ = \frac{1}{\sqrt{L}} \sum_j u_{m,j}(k,0)c_j^†|0⟩.$$

(S10)

The time-evolution is governed by the time-dependent Schrodinger equation, $i\hbar \frac{∂}{∂t}|ψ(t)⟩ = \hat{H}(t)|ψ(t)⟩$. During the pumping process, as the band gap is never closed, the particle will stay in the initial band under adiabatic evolutions. The wave function $|ψ(t)⟩$ at time $t$ can be expanded in the basis of instantaneous Bloch states of the $m$-th band,

$$|ψ(t)⟩ = \sum_k \exp \left(-\frac{i}{\hbar} \int_0^t dt' E_m(k,t')g_k(t)|ψ_m(k,t)⟩,$$

(S11)

where the coefficients $g_k(t)$ satisfy

$$\frac{∂}{∂t} g_k(t) = -\sum_{k'} g_{k'}(t)⟨ψ_m(k,t)|\frac{∂}{∂t}|ψ_m(k',t)⟩$$

$$\times \exp \left(-\frac{i}{\hbar} \int_0^t dt'|E_m(k',t') - E_m(k,t')\right),$$

(S12)
with $g_k(0) = \frac{1}{\sqrt{E}} e^{-ikqR}$. The instantaneous Bloch states are also eigenstates of the translation operator $\hat{T}$

$$\hat{T}|\psi_m(k',t)\rangle = e^{-ik'q}|\psi_m(k',t)\rangle.$$  \hfill (S13)

Here $\hat{T}$ also satisfies $\hat{T}c_j^\dagger |0\rangle = e_j^\dagger |0\rangle$. By differentiating Eq. (S13) and taking scalar product with $\langle \psi_m(k,t) |$, we get

$$(e^{-ik'q} - e^{-ikq})\langle \psi_m(k,t) | \frac{\partial}{\partial t}|\psi_m(k,t)\rangle = 0.$$

(S14)

It means that

$$\langle \psi_m(k,t) | \frac{\partial}{\partial t}|\psi_m(k,t)\rangle = \delta_{k,k'} \langle \psi_m(k,t) | \frac{\partial}{\partial t}|\psi_m(k,t)\rangle.$$  \hfill (S15)

After a pumping cycle ($t = T$), the wave function reads

$$|W_m(R,T)\rangle = \frac{1}{\sqrt{L}} \sum_k e^{-ikqR} e^{i\gamma(k)} |\psi_m(k,0)\rangle,$$  \hfill (S16)

with

$$\gamma(k) = \int_0^T \left( \langle u_m(k,t) | \frac{i}{\hbar} \frac{\partial}{\partial t} | u_m(k,t) \rangle - E_m(k,t) \right) dt = \gamma_b(k) + \gamma_d(k).$$  \hfill (S17)

Here, we respectively denote $\gamma_b$ and $\gamma_d$ as the Berry phase and the dynamical phase. The mean position at $t = T$ is given as

$$\langle \hat{X}_m(T) \rangle = qR - \frac{1}{L} \sum_k \frac{\partial}{\partial k} \gamma(k) + \frac{1}{L} \sum_k \langle u_m(k,0) | i \frac{\partial}{\partial k} | u_m(k,0) \rangle.$$  \hfill (S18)

FIG. S3. (color online). $X_d(k)$ (left) and $X_b(k)$ (right) for the highest band. The parameters are set as the ones for Fig.1 in the main text.

In the limit of large $L$, one can use the form of continuous integral to replace the summation over the quasi-momentum $k$, and the mean position shift in one pumping cycle is given as

$$\Delta P = \langle \hat{X}_m(T) \rangle - \langle \hat{X}_m(0) \rangle.$$
Since $E_m(k, t)$ is periodic with the period $2\pi/q$, the term $\frac{q}{2\pi} \int_{-\pi/q}^{\pi/q} \frac{\partial}{\partial k} \gamma(k) dk$ vanishes. In Fig. S3, we plot $X_d(k) = -\frac{\partial}{\partial k} \gamma_d(k)$ and $X_b(k) = -\frac{\partial}{\partial k} \gamma_b(k)$ versus the quasi-momentum $k$. It is shown that the average value of $X_d(k)$ vanishes and the one of $X_b(k)$ is $qC_m$. This well agrees with the analytical value given by Eq. (S19).

**Variation of diffusion width during Thouless pumping**

From the definition of the spread functional $\Omega$ and the diffusion width $D_W$, we know that $D_W = \sqrt{\Omega}$. To get the variation of $D_W$, we analyze the spread functional first. For the isolated band we consider, the spread functional of the Wannier states in the $m$-th band can be written as

$$
\Omega(t) = |\langle W_m(0, t)| \hat{X}^2 |W_m(0, t)\rangle - \langle W_m(0, t) | \hat{X} |W_m(0, t)\rangle|^2
$$

$$
= \langle W_m(0, t) | \hat{X} \left( \sum_{m', R} [W_{m'}(R, t)] \langle W_{m'}(R, t) | \hat{X} |W_m(0, t)\rangle - \langle W_m(0, t) | \hat{X} |W_m(0, t)\rangle \right) \rangle^2
$$

$$
= \sum_{m' \neq m, R} |\langle W_{m'}(R, t) | \hat{X} |W_m(0, t)\rangle|^2 + \sum_{R \neq 0} |\langle W_m(R, t) | \hat{X} |W_m(0, t)\rangle|^2.
$$

It can be decomposed as two terms, $\Omega = \Omega_I + \Omega_D$, with

$$
\Omega_I = \sum_{m' \neq m, R} |\langle W_{m'}(R, t) | \hat{X} |W_m(0, t)\rangle|^2,
$$

$$
\Omega_D = \sum_{R \neq 0} |\langle W_m(R, t) | \hat{X} |W_m(0, t)\rangle|^2.
$$

Here, $\Omega_I$ is gauge invariant and therefore doesn’t change during the whole pumping procedure, and $\Omega_D$ is zero for the MLWSs [1–3].

We now turn to calculate $\Omega_D$ at time $T$. To do this, we calculate the elements $\langle W_m(R, T) | \hat{X} |W_m(0, T)\rangle$ and obtain

$$
\langle W_m(R, T) | \hat{X} |W_m(0, T)\rangle
$$

$$
= \frac{1}{L} \sum_{k, k', j} e^{i(k-k')qR} e^{i(k-k')\gamma(k')} e^{i(k-k')u_{m, j}(k', 0)} \left( -\frac{\partial}{\partial k} \gamma(k) \right) u_{m, j}(k, 0) + i \frac{\partial}{\partial k} u_{m, j}(k, 0)
$$

$$
= \frac{1}{L} \sum_k e^{ikqR} \left( \langle u_m(k, 0) | i \frac{\partial}{\partial k} |u_m(k, 0)\rangle - \frac{\partial}{\partial k} \gamma(k) \right),
$$

The derivation of Eq. (S22) is similar to Eq. (S9). Thus we get

$$
\Omega_D(T) = \sum_R |\langle W_m(R, T) | \hat{X} |W_m(0, T)\rangle|^2 - |\langle W_m(0, T) | \hat{X} |W_m(0, T)\rangle|^2
$$

$$
= \frac{1}{L^2} \sum_{R, k, k'} e^{i(k-k')qR} \left( \langle u_m(k, 0) | i \frac{\partial}{\partial k} |u_m(k, 0)\rangle - \frac{\partial}{\partial k} \gamma(k) \right) \times
$$

$$
\left( \langle u_m(k', 0) | i \frac{\partial}{\partial k} |u_m(k', 0)\rangle - \frac{\partial}{\partial k} \gamma(k') \right) - \frac{1}{L} \sum_k \langle u_m(k, 0) | i \frac{\partial}{\partial k} |u_m(k, 0)\rangle - \frac{\partial}{\partial k} \gamma(k) \right)^2
$$

$$
= \frac{1}{L} \sum_k \left( \langle u_m(k, 0) | i \frac{\partial}{\partial k} |u_m(k, 0)\rangle - \frac{\partial}{\partial k} \gamma(k) \right) - \left( \frac{1}{L} \sum_k \langle u_m(k, 0) | i \frac{\partial}{\partial k} |u_m(k, 0)\rangle - \frac{\partial}{\partial k} \gamma(k) \right)^2
$$

$$
= \frac{1}{L} \sum_k \left[ \langle u_m(k, 0) | i \frac{\partial}{\partial k} |u_m(k, 0)\rangle - \frac{\partial}{\partial k} \gamma(k) \right] - \left( \frac{1}{L} \sum_k \langle u_m(k, 0) | i \frac{\partial}{\partial k} |u_m(k, 0)\rangle - \frac{\partial}{\partial k} \gamma(k) \right)^2
$$
\[ = \frac{1}{L} \sum_k \left( -\frac{\partial}{\partial k} \gamma(k) + \frac{1}{L} \sum_k \frac{\partial}{\partial k} \gamma(k) \right)^2. \]  
(S23)

Here, we use the relation
\[
\langle u_m(k,0)|i\frac{\partial}{\partial k}|u_m(k,0)\rangle = \frac{1}{L} \sum_k \langle u_m(k,0)|i\frac{\partial}{\partial k}|u_m(k,0)\rangle,
\]  
(S24)

for the MLWSs [1–3]. In the limit of large \( L \), we can use the form of continuous integral to replace the summation over quasi-momentum \( k \) and obtain
\[
\Omega_D(T) = \frac{q}{2\pi} \int_{-\pi/q}^{\pi/q} \left( -\frac{\partial}{\partial k} \gamma(k) + \frac{q}{2\pi} \int_{-\pi/q}^{\pi/q} \frac{\partial}{\partial k} \gamma(k) dk \right)^2 dk
\]
\[
= \frac{q}{2\pi} \int_{-\pi/q}^{\pi/q} \left( -\frac{\partial}{\partial k} \gamma(k) - qC_m \right)^2 dk
\]
\[
= \frac{q}{2\pi} \int_{-\pi/q}^{\pi/q} \left( X_d(k) + \xi(k) \right)^2 dk
\]
(S25)

In Fig. S4, we plot \( X_d(k) \) and \( \xi(k) = X_b(k) - qC_m \) versus the quasi-momentum \( k \). It clearly shows that \( X_d(k) \) is the main source of diffusion.

![Fig. S4](image-url)

**FIG. S4.** (color online). \( X_d(k) \) (blue solid line) and \( \xi(k) \) (red dotted line) for the highest band. The parameters are set as the ones for Fig.1 in the main text.

**Effective Hamiltonian under weak tunnelings**

Under strongly diagonal modulation (\(|J/V_0| \ll 1\)), we can treat the tunnelings
\[
\hat{V} = \sum_j \left( J_j c_j^\dagger c_{j+1} + \text{H.c.} \right),
\]  
(S26)

as a perturbation to the on-site potentials
\[
\hat{H}_0 = \sum_j V_j c_j^\dagger c_j.
\]  
(S27)
As shown in the main text, we can decompose a pumping cycle into three regions: I, II and III. The unperturbed term $\hat{H}_0$ has three eigenvalues, $E_1 = V_A$, $E_2 = V_B$, and $E_3 = V_C$ each with the $L$-fold degenerate eigenstates. As an example, we calculate the effective Hamiltonian for region I, where $V_A$ and $V_B$ are far separated from $V_C$. The effective Hamiltonians for regions II and III are quite similar and will be given at last. The eigenstates of $\hat{H}_0$ construct two different subspaces: (1) the subspace $\mathcal{U}$ formed by $\{|A\>_l, |B\>_l\}$ (with $l=1,...,L$), and (2) the subspace $\mathcal{V}$ formed by $\{|C\>_l\}$ (with $l=1,...,L$). The projection operators on spaces $\mathcal{U}$ and $\mathcal{V}$ are respectively defined as

$$P_0 = \sum_l |A\>_l \langle A| + |B\>_l \langle B|,$$

$$Q_0 = \sum_l |C\>_l \langle C|.$$  \hspace{1cm} (S28)

According to the degenerate perturbation theory [4, 5], the effective Hamiltonian (up to the third-order) for the subspace $\mathcal{U}$ is given as

$$\hat{H}_U = \hat{H}_0 P_0 + P_0 \hat{V} P_0 + \frac{1}{2} P_0 [S_1, V_{od}] P_0 + \frac{1}{2} P_0 [S_2, V_{od}] P_0,$$  \hspace{1cm} (S29)

with

$$S_1 = \mathcal{L}(V_{od}), \quad S_2 = -\mathcal{L}([V_d, S_1])$$

$$V_d = \mathcal{D}(\hat{V}), \quad V_{od} = \mathcal{O}(\hat{V}).$$ \hspace{1cm} (S30)

Here, the super-operators are defined as

$$\mathcal{O}(\hat{Y}) = P_0 \hat{Y} Q_0 + Q_0 \hat{Y} P_0,$$

$$\mathcal{D}(\hat{Y}) = P_0 \hat{Y} P_0 + Q_0 \hat{Y} Q_0,$$

$$\mathcal{L}(\hat{Y}) = \sum_{i,j} \frac{\langle i| \mathcal{O}(\hat{Y}) | j\rangle}{E_i - E_j} |i\rangle \langle j|.$$ \hspace{1cm} (S31)

with $\{|i\rangle\}$ be an orthonormal eigenbasis of $\hat{H}_0$ and $\hat{H}_0 |i\rangle = E_i |i\rangle$ for all $i$. We denote the eigenvalues and eigenstates belonging to the subspace $\mathcal{U}$ as $\{E_{l0}\}$ and $|l0\rangle$, respectively. The first-order expansion is given as $P_0 \hat{V} P_0$. The second-and third-order expansion respectively read as

$$P_0 [S_1, V_{od}] P_0 = \sum_{i,j \in l_0, m \notin l_0} \left[ \frac{1}{E_i - E_m} + \frac{1}{E_j - E_m} \right] \langle i| \hat{V} |m\rangle \langle m| \hat{V} |j\rangle |i\rangle \langle j|,$$ \hspace{1cm} (S32)

and

$$P_0 [S_2, V_{od}] P_0 = \sum_{i,j \in l_0, m \notin l_0} \langle j| \hat{V} |m\rangle \langle m| \hat{V} |n\rangle \langle n| \hat{V} |i\rangle \langle i| |j\rangle$$

$$+ \sum_{i,j \in l_0, m \notin l_0} \langle i| \hat{V} |m\rangle \langle m| \hat{V} |n\rangle \langle n| \hat{V} |j\rangle \langle j| |i\rangle$$

$$- \sum_{i,j,k \in l_0, m \notin l_0} \langle k| \hat{V} |m\rangle \langle m| \hat{V} |i\rangle \langle i| \hat{V} |j\rangle \langle j| |k\rangle$$

$$- \sum_{i,j,k \in l_0, m \notin l_0} \langle j| \hat{V} |i\rangle \langle i| \hat{V} |m\rangle \langle m| \hat{V} |k\rangle \langle k| |j\rangle.$$ \hspace{1cm} (S33)

Similarly, the effective Hamiltonian for the subspace $\mathcal{V}$ can also be obtained and the total effective Hamiltonian for region I read as

$$\hat{H}_I = \sum_l V_{lA} c_{l,A} c_{l,A}^\dagger + V_{lB} c_{l,B} c_{l,B}^\dagger + V_{lC} c_{l,C} c_{l,C}^\dagger + J_1^{(1)} c_{l,A}^\dagger c_{l,B} c_{l-1,B} + J_1^{(2)} c_{l,A} c_{l-1,B}$$
The effective Hamiltonian for one pumping cycle is given as

\[ -J_1^{(3)} \left( c_{i,A}^\dagger c_{i+1,A} + c_{i,B}^\dagger c_{i+1,B} - 2c_{i,C}^\dagger c_{i+1,C} \right) + \text{H.c.} \].

(S34)

Where \( V_{1A} = V_A + \frac{J_1^2}{2\Delta_1} \), \( V_{1B} = V_B + \frac{J_1^2}{2\Delta_1} \), and \( V_{1C} = V_C - \frac{J_1^2}{2\Delta_1} - \frac{J_2^2}{2\Delta_2} \) are effective on-site potentials and \( J_1^{(1)} = J_1 - \frac{J_1(J_1^2 + J_2^2)}{4\Delta_1\Delta_1} \), \( J_1^{(2)} = \frac{J_2J_1}{2\Delta_1} (\frac{1}{\Delta_1} + \frac{1}{\Delta_2}) \), and \( J_1^{(3)} = \frac{J_2J_1}{2\Delta_1\Delta_2} \) are respectively the first-, second-, and third-order tunneling strengths. Here \( J_1, J_2, \) and \( J_3 \) are respectively the tunneling strengths between \( A \) and \( B, B \) and \( C \) in the same cell, and \( C \) and \( A \) in two nearest neighbouring cells. The potential biases are denoted as \( \Delta_1 = V_A - V_B, \Delta_2 = V_B - V_C, \Delta_3 = V_A - V_C \).

The effective Hamiltonian for one pumping cycle is given as

\[ \hat{H}_{\text{eff}} = \begin{cases} \hat{H}_1, & \phi(t) \in [0, \pi/6) \cup [5\pi/6, 7\pi/6) \cup [11\pi/6, 2\pi] \\ \hat{H}_{\text{II}}, & \phi(t) \in [\pi/6, \pi/2) \cup [7\pi/6, 3\pi/2) \\ \hat{H}_{\text{III}}, & \phi(t) \in [\pi/2, 5\pi/6) \cup [3\pi/2, 11\pi/6) \end{cases} \] (S35)

with \( \hat{H}_1 \) given in (S34) and

\[ \hat{H}_{\text{II}} = \sum_{l} V_{1A} c_{l,A}^\dagger c_{l,A} + V_{1B} c_{l,B}^\dagger c_{l,B} + V_{1C} c_{l,C}^\dagger c_{l,C} + J_1^{(1)} c_{l,B}^\dagger c_{l-1,B} c_{l-1,B} c_{l,B} + J_1^{(3)} (c_{l,B}^\dagger c_{l+1,B} c_{l,B} + c_{l,B} c_{l+1,B}^\dagger) + \text{H.c.} \]

\[ \hat{H}_{\text{III}} = \sum_{l} V_{1A} c_{l,A}^\dagger c_{l,A} + V_{1B} c_{l,B}^\dagger c_{l,B} + V_{1C} c_{l,C}^\dagger c_{l,C} + J_1^{(1)} c_{l,A}^\dagger c_{l+1,A} c_{l+1,A} c_{l,A} - 2c_{l,B}^\dagger c_{l+1,B} c_{l,B} + c_{l,C}^\dagger c_{l+1,C} c_{l,C} + \text{H.c.} \] (S36)

Where \( V_{1A} = V_A + \frac{J_2^2}{2\Delta_1} \), \( V_{1B} = V_B - \frac{J_2^2}{2\Delta_1} \), \( V_{1C} = V_C - \frac{J_2^2}{2\Delta_1} + \frac{J_2^2}{2\Delta_2} \), \( J_1^{(1)} = J_2 - \frac{J_2^2}{2\Delta_1\Delta_1} \), \( J_1^{(2)} = \frac{J_2^2}{2\Delta_1\Delta_2} \), \( J_1^{(3)} = \frac{J_2^2}{2\Delta_2} \), and \( V_{1IA} = V_A + \frac{J_2^2}{\Delta_1^2} \), \( V_{1IB} = V_B - \frac{J_2^2}{\Delta_1^2} + \frac{J_2^2}{\Delta_2^2} \), \( V_{1IC} = V_C - \frac{J_2^2}{\Delta_1^2} + \frac{J_2^2}{\Delta_2^2} \), \( J_{1IA} = J_3 - \frac{J_3^2}{2\Delta_1\Delta_1} \), \( J_{1IB} = \frac{J_3^2}{2\Delta_1\Delta_2} \), \( J_{1IC} = \frac{J_3^2}{2\Delta_2^2} \).

FIG. S5. (color online). Thouless pumping during one pumping cycle. Left: the density distribution \( \langle \hat{n}_j \rangle \). Right: the mean position shift \( \Delta P \) and the diffusion width \( D_W \). (a) and (b) respectively correspond to the original and effective Hamiltonians. The parameters are set as the ones for Fig.1 in the main text.

In Fig. S5, we compare the Thouless pumping under the original Hamiltonian (Eq. (1) in the main text) and the effective Hamiltonian \( \hat{H}_{\text{eff}} \) (Eq. (S35)). Clearly, the results obtained from the effective Hamiltonian are agree with those obtained from the original Hamiltonian.
FIG. S6. (color online). Flatness ratios during one pumping cycle with fixed tunneling strengths (a) and with modulated ones (b). The solid, dotted and dashed lines respectively correspond to the lowest, middle and highest bands. The parameters are set as the ones for Fig.1 in the main text.

In high-order tunneling suppression protocol, we modulate the nearest neighbouring tunneling strengths based on the on-site potential bias. This modulation suppresses the effectively high-order tunnelings and we find it also makes the Bloch band more flat. The energy gap between the $m$-th and $(m+1)$-th bands is defined as $G_m = \min_{k\{k\}} (E_{m+1,k} - E_{m,k})$. The bandwidth for $m$-th band is defined as $W_m = \max_{k\{k\}} (E_{m,k} - \min_k E_{m,k})$. The flatness ratios for our three-band system are respectively given as $\delta_1 = W_1/G_1$, $\delta_2 = W_2/\min(G_1, G_2)$, and $\delta_3 = W_3/G_2$. In Fig. S6, we show the flatness ratios with respect to the time-dependent phase $\phi(t)$.

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