Experimental Observation of a Generalized Thouless Pump with a Single Spin

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Adiabatic cyclic modulation of a one-dimensional periodic potential will result in quantized charge transport. Such a pump is termed the Thouless pump. In contrast to the original Thouless pump restricted by the topology of the parameter space, here we experimentally observe a generalized Thouless pump that can be extensively and continuously controlled. The extraordinary features of the new pump originate from interband coherence in nonequilibrium initial states, and this fact indicates that a quantum superposition of different eigenstates individually undergoing quantum adiabatic following can also be an important ingredient unavailable in classical physics. Additionally, because the pumping is most pronounced around a band-touching point, this work also offers a nonequilibrium means to detect quantum or topological phase transitions. The quantum simulation of this generalized Thouless pump in a two-band insulator is achieved by applying delicate control fields to a single spin in diamond. The experimental results demonstrate all principal characteristics of the generalized Thouless pump.

In 1983, Thouless discovered that the charge transport across a one-dimensional lattice over an adiabatic cyclic variation of the lattice potential is quantized, equaling to the Chern number defined over a two-dimensional Brillouin zone formed by quasimomentum and time [1]. This phenomenon, known as the topological charge pump or Thouless pump, shares the same topological origin as the quantization of Hall conductivity [2–4] and may thus be regarded as a dynamical version of the integer quantum Hall effect [5]. In the ensuing years, the theory of the Thouless pump was investigated extensively [4]. Up to now, several single-particle pumping experiments have been implemented in nanoscale devices [6–9]. Most recently, the topological Thouless pump was observed in cold atom systems [10, 11]. On the application side, the Thouless pump has the potential for realizing novel current standards [12, 13], characterizing many-body systems [14–18], and exploring higher dimensional physics [19].

In Thouless’ original proposal and almost all the follow-up researches, the initial-state quantum coherence between different energy bands, namely, the interband coherence in the initial states, is not taken into account. As a fundamental feature of quantum systems [20, 21], quantum coherence is at the root of a number of fascinating phenomena in chemical physics [22–24], quantum optics [25–28], quantum information [29], quantum metrology [30–32], solid-state physics [33, 34], thermodynamics [35–39], and even biology [40–42]. Therefore, a question naturally arises as to how the pump will behave if the interband coherence resides in the initial state. In this work, we generalize the Thouless pump by incorporating the interband coherence into the initial state, and hence present a quantum adiabatic pump distinct from the conventional Thouless pump.

The effect of the interband coherence in the initial state can be preliminarily evaluated by taking a qualitative analysis of the quantum adiabatic evolution. For the initial states without interband coherence, the cyclic adiabatic operation of duration $T$ induces a population correction of the order $1/T^2$ and an interband coherence of the order $1/T$. These nonadiabatic effects, albeit vanishing in the adiabatic limit, are crucial to yield the quantized transport determined by a weighted integral of the Berry curvature [1, 4]. However, for adiabatic following of superposition states, the interband coherence in the initial states generically induce a population correction of the order $1/T$ to each band, in contrast to the usual $1/T^2$ population correction (see Fig. 1). This underlying mechanism indicates that if a quantum system accommodates interband coherence from the very start as a quantum resource, then the ensuing pumping may have unforeseen features. Intriguingly, the amount of transported charges contributed from the initial interband coherence is found to be finite in the adiabatic limit, namely, $T \to \infty$. In particular, in contrast to the original quantized Thouless pump subjected to the topology, the generalized Thouless pump fueled by interband coherence can be continuously and extensively controlled by varying the switching-on rate of a pumping protocol. The feature of tunability is reminiscent of the famous Archimedes screw, where water is pumped via rotating a screw-shaped blade in a cylinder and the amount of pumped water can also be changed continuously [43–45]. Furthermore, the generalized Thouless pump is even more efficient around a band-touching point, thus offering a nonequilibrium means to detect quantum and topological phase transitions.

Consider a one-dimensional two-band insulator model...
subject to an adiabatic cyclic manipulation. In the momentum $(k)$ space, the insulator’s Hamiltonian slowly modulated with time is given by

$$H(k, \tau) = \frac{\omega \sin(k)}{2} \left\{ \cos[\phi(\tau)] \sigma_x + \sin[\phi(\tau)] \sigma_y \right\} + \frac{\delta_1 \cos(k) + \delta_2}{2} \sigma_z,$$

(1)

where $\tau = t/T \in [0, 1]$ is the scaled dimensionless time, and $\sigma_{x,y,z}$ are standard Pauli matrices. Throughout this paper, we take $\hbar = 1$. The instantaneous spectrum of $H(k, \tau)$ is gapless at $k = 0$ ($k = \pi$) when $\delta_1 = -\delta_2$ ($\delta_1 = \delta_2$). An adiabatic cycle can be realized by slowly varying $\phi$ from 0 to $2\pi$. For a general initial state with reflection-symmetric populations in $k$, the pumped amount of charge $Q$ over one adiabatic cycle can then be found from the first-order adiabatic perturbation theory [46–49]. Specifically, in the adiabatic limit ($T \rightarrow \infty$), the charge transport can be decomposed as $Q = Q_{\text{EQ}} + Q_{\text{IBC}} + Q_{\text{TS}}$, with

$$Q_{\text{EQ}} = \frac{1}{2\pi} \int_{-\pi}^{\pi} dk \sum_n \rho_{nn}|_{\tau=0} \int_0^1 d\tau \Omega^{(n)}_{\tau k},$$

(2)

$$Q_{\text{IBC}} = \frac{1}{2\pi} \int_{-\pi}^{\pi} dk \sum_{m,n(m<n)} 2 \text{Im} \left( \frac{\rho_{mn} \langle n | \partial_\tau | m \rangle}{E_m - E_n} \right) \int_0^1 d\tau (v_{mm} - v_{nn}),$$

(3)

and $Q_{\text{TS}}$ originating from some transient effects associated with the initial state. Here $m$ and $n$ are band indices, states $|m(k, \tau)\rangle$ represent instantaneous eigenstates of $H(k, \tau)$ with eigenvalue $E_m(k)$, $\rho_{mn}(k, \tau)$ and $v_{nm}(k, \tau)$ refer to matrix elements of the density operator and the velocity operator $v(k, \tau) \equiv \partial_\tau H(k, \tau)$ in representation of $|m(k, \tau)\rangle$, and $\Omega^{(n)}_{\tau k}$ is the Berry curvature of the $n$th instantaneous energy band of $H(k, \tau)$. The term $Q_{\text{TS}}$ is of least interest because it does not accumulate with the number of pumping cycles and independent of any aspect of a pumping protocol (see Supplemental Material [50]). The pumping component $Q_{\text{EQ}}$ represents a weighted integral of the Berry curvature, as found previously by Thouless [1]. The pumping component $Q_{\text{IBC}}$, namely, the charge pumping induced by interband coherence in the initial state, is responsible for the generalized Thouless pump and will be the focus of our experimental study below. Because the initial state considered here is always symmetric in $k$, $Q_{\text{IBC}}$ is unrelated to any symmetry breaking of the initial state. Rather, analogous to the conventional Thouless pumping, it arises from an accumulation of small nonadiabatic effects during the pumping. Note that $Q_{\text{IBC}}$ derived in the adiabatic limit ($T \rightarrow \infty$) diverges at quantum or topological phase transition points where the two bands touch each other. However, in actual experiments the duration $T$ of an adiabatic cycle is always finite and hence there is no true divergence in physical observations.

The generalized Thouless pump can be experimentally realized on a qubit system because the insulator’s Hamiltonian in Eq. (1) is also the Hamiltonian of a qubit in a rotating field, we can experimentally demonstrate the generalized Thouless pump using a single spin [51]. To highlight the contribution from $Q_{\text{IBC}}$, in our experiment the initial state is properly designed such that $Q_{\text{EQ}} = Q_{\text{TS}} = 0$, i.e., the traditional Thouless pumping and the initial transient effect have no contribution. To demonstrate the sensitivity of $Q_{\text{IBC}}$ to the switching-on rate of the pumping protocol, namely, $\frac{d\phi(\tau)}{d\tau}|_{\tau=0}$, we consider two different adiabatic protocols with $\phi(\tau) = 2\pi \tau$ and $\phi(\tau) = 2\pi \tau^2$. The first protocol depicts a linear ramp, whereas the second depicts a quadratic ramp with a vanishing switching-on rate at $\tau = 0$. Because $Q_{\text{IBC}}$ is proportional to the term $\langle m | \partial_\tau | n \rangle \sim \frac{d\phi(\tau)}{d\tau}|_{\tau=0}$, one directly sees that the latter choice with zero switching-on rate will make $Q_{\text{IBC}} = 0$ in theory (within the first-order adiabatic perturbation theory). This fact is used in our experiment to not only achieve the tunability inherent in the generalized Thouless pump, but also confirm the negligible role of $Q_{\text{TS}}$. In our experiment, we use a negatively charged nitrogen-vacancy (NV) center in diamond. The single spins in NV centers are convenient to initialize and read out, have long coherence time, and can be manipulated with high precision. Indeed, due to these advantages NV centers are one main platform in studies of nanoscale sensing, quantum information, and fundamen-
The diamond we use is a bulk sample with the $^{13}$C nuclide at the natural abundance of about 1.1% and the nitrogen impurity less than 5 ppb. The NV center is composed of one substitutional nitrogen atom and an adjacent vacancy as shown in Fig. 2(a). Under an external magnetic field parallel to the symmetry axis of the NV center, the electronic ground state $^3A_2$, which is a triplet state, can be described by the Hamiltonian $H_{\text{NV}} = DS_z^2 + \gamma BS_z$, where the first term is zero-field splitting with $D = 2\pi \times 2870$ MHz, the second term is Zeeman splitting with the gyromagnetic ratio $\gamma = 2\pi \times 2.80$ MHz/G, $S_z$ is the spin-1 angular momentum operator of the $z$ direction, and $B$ is the magnitude of the magnetic field. In our experiment, the external static magnetic field is along the NV symmetry axis with the magnitude $B \approx 510$ G. Such magnetic field enables both the NV electron spin and the host $^{14}$N nuclear spin to be polarized by optical excitation [56, 57]. As illustrated in Fig. 2(b), microwave generated by an arbitrary waveform generator drives the transition between the two levels $|m_s = 0\rangle$ and $|m_s = -1\rangle$ which compose a qubit, and the level $|m_s = 1\rangle$ remains idle due to large detuning. The spin state can be read out by optical excitation and red fluorescence detection. All the optics is performed on a home-built confocal microscope, and a solid immersion lens is etched on the diamond above the NV center to enhance the fluorescence collection [58, 59].

In the experiment, the Hamiltonian in Eq. (1) is constructed in the rotating frame with the rotation angular frequency $\omega_0 - \delta_1 \cos k - \delta_2$ where $\omega_0 = D - \gamma B$ is the resonant frequency of the qubit (see Supplemental Material [50]). All our descriptions below are in this rotating frame. We work with $\omega = 2\pi \times 20$ MHz and $\delta_1 = 2\pi \times 10$ MHz, and select several frequencies between 0 to $2\pi \times 20$ MHz for $\delta_2$. In order to obtain the pumped charge $Q$ for each value of $\delta_2/\delta_1$, the double integral of the velocity expectation value over the first Brillouin zone needs to be evaluated. Since the pumped charge contributed from a certain $k$, namely, $q(k) = T \int_0^1 \langle v(k, \tau) \rangle d\tau$, is independent of each other, they are measured separately in different runs of experiment. The pulse sequence for each $k$ is sketched in Fig. 2(c). At first the qubit is polarized to the state $\rho_0 = (1 + \sigma_z)/2$ by a green laser pulse, and then the initial state $\rho(k, 0)$ is prepared by a resonant microwave pulse. From Eq. (3) one can see that $Q_{\text{IBC}}$ might be small if the off-diagonal matrix elements $\rho_{mn}(k, 0)$ associated with different $k$ are chosen without design. To maximize $Q_{\text{IBC}}$ in the experiment, $\rho(k, 0)$ are properly prepared as depicted in Fig. 2(c) [60]. As elucidated in Supplemental Material [50], such initial states also make $Q_{\text{EQ}}$ and $Q_{\text{TS}}$ vanish. Once the preparation of $\rho(k, 0)$ is done, the qubit is subjected to the Hamiltonian $H(k, \tau)$. The evolution governed by $H(k, \tau)$ lasts for some duration $\tau_e \in [0, \tau]$, during which the angle $\phi$ increases coherently according to a pumping protocol.

Immediately after the evolution, one needs to measure the velocity $v(k, \tau_e)$. As shown in Fig. 2(c), the measurement comprises two steps, namely, a resonant microwave pulse and the subsequent laser illumination. The combined effect of the two steps amounts to the observation of $v(k, \tau_e)/\|v\|$, where $\|v\|$ is the spectral norm of $v$ and is time-independent. The above sequence is performed for a series of $\tau_e$ between 0 and 1, and is repeated at least a hundred thousand times to obtain the expectation value. One can then have $\langle v(k, \tau) \rangle/\|v\|$ as a function of $\tau$. Numerical integration over $\tau$ based on experimental data for discrete values of $\tau_e$, multiplied by $\|v\|$, yields the experimental value of $q(k)$. This procedure is repeated for different values of $k \in [0, \pi]$. As detailed in Supplemental Material [50], it suffices to let our measurements cover half of the first Brillouin zone to compare with theory. Some experimental data with $T = 1$ µs and $\phi(\tau) = 2\pi\tau$ are instantiated in Fig. 3. The pattern of the normalized velocity $\langle v(k, \tau) \rangle/\|v\|$ depends strongly on $\delta_2/\delta_1$, and so does the shape of $q(k)$. In particular, there is a significant charge transport for $\delta_2/\delta_1 \approx 1$ and $k \approx \pi$, i.e., near the band touching point.

The integral of $q(k)$ over $k \in [0, \pi]$ yields the total physics [52–55].
charge $Q = \int_{-\pi}^{\pi} q(k) \frac{dk}{(2\pi)} = \int_{0}^{\pi} q(k) \frac{dk}{\pi}$ thanks to a reflection symmetry $\langle v(k, \tau) \rangle = \langle v(-k, \tau) \rangle$ for the specific initial states we choose. As illustrated by the orange curve and data points in Fig. 4(a), the pumped charge $Q$ first rises and then declines as the parameter $\delta_2/\delta_1$ sweeps from 0 to 2. Though the ramp time $T = 1 \, \mu s$ is still not in the true adiabatic limit $T \to \infty$, the pumped charge $Q$ as a function of $\delta_2/\delta_1$ bears strong resemblance with the theoretical curve for $T \to \infty$, with their differences well accounted for. In particular, because a diverging $Q$ at $\delta_2/\delta_1 = 1$ occurs only for $T \to \infty$, the observed pumping for a finite $T = 1 \, \mu s$ is not expected to shoot to infinity. The peak of $Q$ is not precisely at $\delta_2/\delta_1 = 1$, but has a rightward shift. In this linear ramp case, a non-perturbative theory can be developed (see Supplemental Material [50]). The theoretical shift of the peak of $Q$ as a function of $\delta_2/\delta_1$ is found to be $2\pi/(\delta_1 T)$, in good agreement with our observation. This clearly indicates that the observed peak shift is merely a finite-$T$ effect. For a shorter ramp time $T = 0.5 \, \mu s$ as depicted by the green curve and data points in Fig. 4(a), the pumping peak slightly goes lower again and shifts further away from the exact phase transition point $\delta_2/\delta_1 = 1$. Overall, the two pumping curves with $T = 1.0 \, \mu s$ and $T = 0.5 \, \mu s$ have a remarkable overlap with each other, thus sup-
porting that to the zeroth order, the outcome of the generalized Thouless pump is independent of $T$. We next investigate another pumping protocol $\phi(\tau) = 2\pi\tau^2$ with $T = 1 \mu s$. The initial switching-on rate of this pumping protocol now vanishes. In this case, we observe negligible pumping, as evidenced by the blue curve and data points in Fig. 4(a). The results for the second protocol confirm that the generalized Thouless pump can be extensively tuned by varying the switching-on rate of a pumping protocol. Finally, one may note the differences between experimental results and the simulation results (smooth orange, green, and blue curves in Fig. 4(a)] based solely on time-dependent Schrödinger equations. The experimental errors are mainly due to the imperfection of the microwave pulses. Nevertheless, in the presence of the unavoidable experimental errors, our experimental results have demonstrated all principal features of the generalized Thouless pump.

In conclusion, by incorporating interband coherence into the initial state as a powerful quantum resource, we are able to go beyond the traditional Thouless adiabatic pump. Using a single spin in diamond, we have experimentally demonstrated a novel type of quantum adiabatic pump, which is extensively and continuously tunable by varying the switching-on rate of a pumping protocol. The experimental results have also confirmed our theoretical findings [48, 49]. This work establishes a new means for the detection of band-touching and hence quantum or topological phase transition points, and enriches the physics of adiabatic pump and coherence-based quantum control.

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n = \frac{(-\delta_1 \cos k - \delta_2, 0, \omega \sin k)}{\sqrt{(\omega \sin k)^2 + (\delta_1 \cos k + \delta_2)^2}}.
\]
The Bloch vector \( \mathbf{n} \) lies in the \( xz \) plane and is perpendicular to the field. In the singular case where \( \delta_1 = \delta_2 \) and \( k = \pi \), the Bloch vector \( \mathbf{n} \) is defined as

\[
\mathbf{n}\big|_{\delta_1=\delta_2,k=\pi} = \lim_{k\to\pi} \frac{(-\delta_1 \cos k - \delta_2, 0, \omega \sin k)}{\sqrt{(\omega \sin k)^2 + (\delta_1 \cos k + \delta_2)^2}} \bigg|_{\delta_1=\delta_2}
\]

\[
= (0, 0, 1).
\]

Such initial states maximize \( Q_{\text{IBC}} \), and eliminate \( Q_{\text{TS}} \) and \( Q_{\text{EQ}} \).