Correlation-Assisted Quantized Charge Pumping

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We investigate charge pumping in the vicinity of order-obstructed topological phases, i.e. symmetry protected topological phases masked by spontaneous symmetry breaking in the presence of strong correlations. To explore this, we study a prototypical Su-Schrieffer-Heeger model with finite-range interaction that gives rise to orbital charge density wave order, and characterize the impact of this order on the model’s topological properties. In the ordered phase, where the many-body topological invariant loses quantization, we find that not only is quantized charge pumping still possible, but it is even assisted by the collective nature of the orbital charge density wave order. Remarkably, we show that the Thouless pump scenario may be used to uncover the underlying topology of order-obstructed phases.

The robust quantization of transport properties observed in topological states of quantum matter is among the most fascinating phenomena in physics [1, 2], both from a fundamental perspective and due to its far-ranging potential for technological applications [3–5]. A primary example along these lines is provided by the integer quantum Hall effect [6, 7] in two-dimensional systems with a finite Chern number [8], as induced by a strong perpendicular magnetic field. Seminal work by Laughlin [9] and Thouless [10] has revealed that this topologically quantized charge transport may be understood as a cyclic adiabatic pumping process in time-dependent one-dimensional systems. While these intriguing phenomena can be understood within the independent particle approximation in the framework of topological Bloch bands [2], their stability against imperfections such as disorder and weak to moderate correlations is well established [1, 11, 12]. In strongly correlated systems, however, qualitative changes to this picture occur, including the breakdown of topological band theory due to spontaneous symmetry breaking [13, 14] and dynamical quantum fluctuations [15–17], respectively, but also the formation of genuinely correlated topologically ordered phases [18].

In this work, we demonstrate how spontaneous symmetry breaking can facilitate and even drive quantized charge pumping (see sketch in Fig. 1). Remarkably, by means of unbiased numerical simulations, we show that this mechanism survives even in a strongly correlated regime, where an effective single-particle picture is found to break down, and would not correctly predict the adiabatic pumping properties. In particular, we observe that the Resta polarization [19] provides an unambiguous many-body topological characterization that agrees with a direct calculation of the relevant transport properties. Furthermore, we reveal how the Thouless charge pumping approach [10, 20] can be used to characterize the buried topological phase diagram of order-obstructed phases, i.e. conventionally ordered phases that arise from symmetry protected topological (SPT) phases [21] by spontaneous symmetry breaking.

To this end, we study in the framework of density matrix renormalization group (DMRG) methods [22, 23] a variant of the Su-Schrieffer-Heeger (SSH) model [24, 25] with finite-range interaction as a conceptually simple system found to exhibit a rich interplay between SPT phases and long-range order. For strong interactions, our model system exhibits an orbital charge-density wave (CDW) which spontaneously breaks the protecting chiral symmetry, thus exemplifying the aforementioned class of order obstructed phases. Our findings closely connect to current experimental activity on realizing topological band structures with ultracold atoms in optical lattices [26–30], and may be verified in a strongly interacting version of recent experiments on quantized charge pumping in such settings [31].

Model and Methods. — Initially conceived as a microscopic description of solitons in polyacetylene [25], the SSH model has become a prototype for topological physics in one-dimensional systems. Several interacting variants of the SSH model have been studied in previous literature [32–34], where

\[ \Delta Q = 0 \]

\[ \Delta Q = 2 \]

FIG. 1. Schematic of correlation-assisted charge pumping. (a): Sketch of correlation-assisted pump cycle in parameter space (solid line) and the effective parameter cycle in the absence of correlations (dashed line). Blue and red background in phase diagram denote orbital character of sublattice ordering (sublattice A and B respectively). (b): Sketch of order parameter over two correlation-assisted pump cycles which do not (upper) and do (lower) pump non-zero charge. Both cycles enter and exit the ordered phase, but only in the bottom cycle, corresponding to the cycle in (a), does the ordering change orbital character, leading to non-zero pumped charge.
on a bipartite chain of spinless fermions with two orbitals per site (a and b). $\hat{a}_j^\dagger (\hat{a}_j)$ and $\hat{b}_j^\dagger (\hat{b}_j)$ represent creation (annihilation) operators on orbitals in sublattice a and b respectively, on site j. $\hat{V}$ is an intra-cell hopping, and $(d \pm \tau)/2$ are alternating inter-cell inter-orbital hopping strengths. In the second summation, $\hat{v}^a = \hat{a}^\dagger \hat{a}$, and likewise for $\hat{v}^b$. To investigate this model, we use the DMRG technique [23], and look at systems with open boundary conditions [38] DMRG and system details are included in the Supplementary Material [39].

To probe topological properties of our model (1), we focus on two many-body topological invariants. First, the Resta (many-body) polarization [19],

$$
P = \frac{q a_0}{2\pi} \text{Im} \ln \text{Tr} \left[ \hat{v} \hat{e}^\frac{\tau}{2} \right] \mod q a_0, \tag{2}
$$

where $a_0$ is the lattice spacing, $L$ is the number of unit cells, and $X = \sum_i x_i \hat{n}_i$ is the many-body center of mass operator; $\hat{p}$ denotes the many-body density matrix [40]. Secondly we study the entanglement spectrum [41–43], which is intimately connected to the Resta polarization [44]. To define this, we consider the reduced density matrix resulting from tracing out one half of our system across a spatial bipartition: $\rho_{KL} = \text{Tr}_R[\rho_{L R}]$. The entanglement spectrum is the set of ordered eigenvalues $\lambda_i$ of the entanglement Hamiltonian $H_{KL} = -\log \rho_{KL}$. The degeneracies of the spectrum are determined by fundamental characteristics of the state, which include topological properties and symmetries such as inversion symmetry. We define the entanglement gap as $\Delta \lambda = \lambda_1 - \lambda_0$.

Phase Diagram. — For concreteness, we focus on the phase diagram slice for $d = 0.4$, $\tau = 1.0$ (cf. Fig. 2 (a)). However, we investigated many parameter combinations and found that the qualitative behavior is generally preserved across the parameter regimes considered. Roughly, increasing $d$ shifts the trivial-topological phase boundary to the right, and $\tau$ does not have much impact on the topological properties (as long as $\tau \neq 0$). Our designations of trivial and topological regions in the phase diagram are determined by the value of the polarization (2) in the normal (symmetric) phase. This is consistent with our aforementioned complementary classification approach by entanglement.

In the resulting phase diagram of the SSH model with interaction (1), we identify four different phases, distinguished by the presence or absence of SPT order and CDW order (see Fig. 2 (a)). The first two phases, band insulator (BI) and topological insulator (TI) are present without interaction and persist for weak to moderate interaction. For sufficiently strong interaction (indicated by the black squares in Fig. 2 (a)), spontaneous orbital CDW order emerges (see [39]), which obstructs the underlying topology. The two resulting phases, OOB1 and OOT1, are characterized by sub-lattice symmetry-breaking. Their topological properties are discussed below. We checked that the phase diagram is not qualitatively changed by the addition of other small terms obeying chiral symmetry, and the presence of a small intra-cell interaction $\hat{U}$. Subsequently, we elaborate on all four phases, going through the phase diagram in Fig. 2 (a) from weak to strong interactions.

For $\hat{V} = 0$, the Hamiltonian can be expressed in the single-particle basis, and all topological information can also be extracted from the single particle density matrix (SPDM) by decomposing $\rho_k(t) = \frac{1}{4} [1 - \mathbf{r}_k(t) \cdot \sigma]$, where $\mathbf{r}_k$ is the pseudospin vector. In equilibrium, the quantity $\nu$, defined by $(-1)^\nu = \text{sgn}(\mathbf{r}_k^T \mathbf{r}_k)$, coincides with the pseudospin winding number [45]:

$$
\nu = \frac{1}{4\pi} \int_{-\pi/\mu}^{\pi/\mu} d\phi \langle \mathbf{n}_k^T \partial_k \mathbf{n}_k \rangle - \langle \mathbf{n}_k^T \partial_k \mathbf{n}_k \rangle, \tag{3}
$$

where $\mathbf{n}_k = \mathbf{r}_k / |\mathbf{r}_k|$. A nontrivial value of either invariant is equivalent to the condition $|d| > |J|$, and a topological phase transition occurs when $|\mathbf{r}_k^T| = 0$, at which point $\nu$ changes sign. One can also view the SPDM as the density matrix corresponding to the mixed state of some auxiliary Hamiltonian, $\rho_k = e^{-\beta \mathbf{h}_k}$ [46], and can use $\mathbf{H}_k$ to compute the Zak phase [47] from its eigenstates: $\zeta = \frac{1}{\pi} \int_{-\pi/\mu}^{\pi/\mu} d\phi \langle \phi_k | \partial_k \phi_k \rangle$. The Zak phase is quantized to $\zeta = \nu$ and can be used as a topological

![FIG. 2. (a): Phase diagram for interacting SSH model with $d = 0.4$, $\tau = 1.0$. TI: Topological Insulator, BI: Band Insulator, OOB1: Order-obstructed Band Insulator, OOT1: Order-obstructed Topological Insulator. Red triangles denote mean field theory results. Black squares denote finite size scaling calculations from fitting the orbital charge density wave phase transition to Ising universality class. Green ‘+’ denote transition points for SPDM topological invariant. Purple diamonds delineate regions of single (right) and double (left) ground state degeneracy. Blue stars denote transition according to polarization in the normal phase. Gradient-filled region in center was numerically unstable. (b): Typical band structures in each phase. Color signifies orbital character, and level of transparency represents strength of band mixing.](image)
invariant in the noninteracting SSH model; it is also equivalent to the quantized polarization, \( P = vqa_0/2 \).

When weak interaction (preserving chiral symmetry) is added to the model, the topological invariant extracted from the SPDM still agrees with the Resta polarization. This reflects the fact that the SPDM still contains most of the information about the many-body topology [39]. The positive slope of the BI \( \rightarrow \) TI phase boundary can be attributed to (even at mean-field level) the interaction pushing the valence and conduction bands closer together, facilitating hybridization. As illustrated in the band-structure sketches in Fig. 2 (b), the TI phase is characterized by band inversion at the \( \Gamma \)-point.

Strong interaction favors the emergence of orbital CDW order with ground states that spontaneously break chiral symmetry. When explicitly suppressing CDW order (thus enforcing chiral symmetry), the blue line in Fig. 2 (a) still separates the topological insulator from the trivial insulator phase. In this scenario, we can distinguish these two phases by their polarization (\( P = 0 \) for trivial, \( P = \pm vqa_0/2 \) for topological) even within the unstable region where in principle charge order would obstruct the SPT phases. Furthermore, the strongly interacting topological region still features edge modes. When allowing for CDW order, the topologically trivial phase defines the OOBI region in Fig. 2 (a) within which no charge can be pumped, and the topological phase defines the OOTI region in Fig. 2 (a), within which quantized charge pumping is possible as shown below.

Nevertheless, even in the order obstructed regime, important signatures of the inherited topological properties persist, as illustrated in Fig. 2 (b). The trivial OOBI has a band structure similar to BI, but with strong band-mixing close to the \( \Gamma \)-point. The band structure of OOTI combines features of TI and OOBI: band inversion and band mixing. The onset of orbital order for transitions TI \( \rightarrow \) OOTI and BI \( \rightarrow \) OOBI can be identified by entanglement signatures in the symmetry-broken state, as we numerically demonstrate in the Supplementary Material [39]. In the band insulating phase, the transition is accompanied by an abrupt change in the slope of the entanglement entropy. In the TI phase, the entanglement gap is \( \Delta \lambda = 0 \), and becomes non-zero upon emergence of orbital order. In the ordered OOTI phase, the edge states are gapped out. Remarkably, even in the presence of CDW order, we will demonstrate that adiabatic charge pumping still allows us to distinguish the OOTI from the OOBI region, as separated by the aforementioned blue phase boundary.

To compare the single-particle and the many-body characterization of the topology, we compute the natural orbitals \( |\phi_k\rangle \) from the SPDM as the best choice of a single-particle basis and the corresponding Zak phase \( Z_{\text{nat}} \). The breakdown of such single-particle topological invariants was previously documented [48]. Remarkably, the Resta polarization \( P \) and \( Z_{\text{nat}} \) agree well for large parts of the phase diagram. In the ordered phase, both \( P \) and \( Z_{\text{nat}} \) fractionalize (Fig. 3 (a)). Although the polarization is not quantized, in the large \( V \) limit, the polarization of the degenerate ground states approaches the fractionalized values \( P = \pm vqa_0/2 \).

However, in the normal phase, where both remain quantized, the Zak phase fails to identify the OOTI \( \rightarrow \) OOBI transition (Fig. 3 (b)) defined by the jump in polarization. The pseudospin winding number similarly misses the OOTI \( \rightarrow \) OOBI transition, as can be seen in the phase diagram (Fig. 2 (a), where all points in parameter-space to the left of the green line have pseudospin winding number \( W = 1 \) and are thus classified as topological by this metric.

**Charge Pumping.** — Despite the fact that the polarization (2) is not quantized in the ordered phase, we find that the underlying topological character of the phase without broken symmetry is present in the adiabatic transport properties of the system. One can imagine adding a (infinitesimally small) staggered on-site potential term \( \tilde{A} = \Delta \sum_{j} (\tilde{\delta}^2_j - \tilde{\delta}^2_j) \) to the model, which acts as a pinning field. The point \( \Delta = \tau = 0 \) is the degeneracy point, at which the system has no preference for either sub-orbitals a or b. Adiabatically looping around this degeneracy point through cyclic variation of \( \Delta \) and \( \tau \), quantized charge

\[
\Delta Q = \frac{1}{a} \int_0^T dt \partial_t P(t),
\]

is transported. In practice, we compute \( P(t) \) along the cycle from the instantaneous Hamiltonian \( \hat{H}(\theta) \) with the loop variable \( \theta \in [0, 2\pi] \).

Inspecting \( \Delta Q \) across the phase diagram Fig. 2, we find that the topological character of the underlying state without broken symmetry is recovered. While this behavior is expected for the weakly-interacting TI phase, it is remarkable that the obstructed OOTI phase (with \( P \neq 0 \) without broken symmetry) is characterized by quantized \( \Delta Q \neq 0 \). This is demonstrated in Fig. 4 (a)–(d).

The unit of quantization in OOTI is 1/2 that of the TI phase, reflecting the fractionalization of excitations in the presence of orbital order. Additionally, while charge is pumped continuously in TI, in OOTI charge is mostly pumped in discrete jumps, driven by the collective order.

These jumps are easily understood in the context of sublattice filling: The cycle begins with the system in the insulating phase. Very abruptly the onset of order leads to orbital occupation supported primarily on sublattice a. This ‘jump’ is
accomplished through shifting half of the electron occupation (the occupation of sub-lattice B orbitals) to the a orbital on the same site. When \( \theta = \pi \), \( \Delta \) changes sign, quickly altering the energy landscape to favor occupation on b rather than a. In this moment, the second jump occurs as all of the electrons shift to the neighboring sublattice b. Finally, the system re-enters the topological insulating phase and half of the occupation moves from b to the a orbital on the same site. Altogether, one unit of charge is pumped during this cycle. Also note that the jump at \( \Delta = \pi \) is twice as large as the other jumps, as all rather than half of the occupation shifts one orbital.

We also note that the single-particle picture of charge pumping breaks down in the presence of strong interactions. An effective single-particle description is obtained from integrating the Berry curvature of the natural orbitals \( \Omega(k,t) = 2 \Im(\partial_i \Phi_b(t)|\partial_i \Phi_a(t)) \): \( \Delta Q = \left(q/2\pi\right) \int dk \int dt \Omega(k,t) n(k,t) \), where \( n(k,t) \) is the larger occupation eigenvalue. Similar to Ref. [44], we find that the non-uniform \( n(k,t) \) along the cycle leads to non-quantized \( \Delta Q \) in this single-particle picture. However, beyond the scenario of a non-uniform momentum distribution discussed in Ref. [44], we find that the Berry curvature description itself breaks down, as evidenced in a discrepancy between Zak phase and Resta polarization for stronger interactions.

Whereas the pump cycles in Fig. 4 (a) and (b) demonstrate that charge pumping remains quantized in the order-obstructed phase, Fig. 4 (c) and (d) illustrate how charge pumping is facilitated by the collective nature of the obstructing order. For these two cycles, there is a critical \( \tau \) that controls whether or not there is orbital ordering when an infinitesimally small seed is added. As such, these cycles utilize the spontaneous symmetry breaking of the ground state to minimize reliance on on-site staggered potential \( \Delta \). In the ordered phase, orbital character of the state is completely determined by the sign of \( \Delta \), independent of magnitude. Thus, one can exert control over the orbital character (for \( \tau \) in the right region) via infinitesimal staggered onsite potential (or any other mechanism which acts as a seed for the order). In (c), both times \( \tau \) becomes small enough to induce ordering it settles on the same orbital character, resulting in net zero charge pumped. In (d) however, \( \Delta \) changes sign, leading to four jumps in sublattice occupation (or two pairs of jumps).

As \( |\tau| \to 0 \), the system spontaneously orders before reaching the degeneracy point, avoiding the band-gap closing [49]. Since this spontaneous ordering randomly picks a direction, not all pump cycles will transport net charge, as demonstrated in Fig. 4 (c). If the sign of the order coincides with that of \( \tau \) as in Fig. 4 (d), then charge is indeed transported. This illustrates the possibility of quantized charge transport with neither bias nor staggered potential.

In this example, the correlation-enhancement to charge pumping comes in the form of eliminating the staggered potential, enabling quantized pumping by only varying the hopping anisotropy. In general, it operationally means one can non-trivially control charge pumping via a single tunable parameter, greatly increasing feasibility of experimental efforts.

Concluding discussion. — In summary, we have described and characterized the effect of spontaneous symmetry-breaking on many-body topology, and have shown that the Thouless pump can be used to identify the underlying topology in order-obstructed phases. Moreover, we illustrate that collective order can be conducive to quantized charge transport, with the spontaneous ordering working to prevent band gap closing even when the model is tuned to the degeneracy point. En route to demonstrating this effect, we have presented a complete phase diagram for an SSH model with non-local interaction, including a phase in which orbital charge density wave order obstructs topology. Our model may be realized in state of the art experiments on cold-atoms in optical lattices [31].

The correlation-assisted charge-pumping we demonstrate in the interacting SSH model should be typical of the interplay between topology and collective order. In our present case of a spontaneously broken \( \mathbb{Z}_2 \) symmetry, random fluctuations alone suffice to produce quantized charge transport. For other symmetries, what survives is that only an infinitesimally small external potential is needed to control transport processes. The collective phase can be exploited to circumvent the many-body
topological constraint in real-time evolution, where the topological invariant is pinned to its initial value under unitary evolution. Hence, a dynamical topological phase transition can be induced by passing through the symmetry-breaking collective phase, giving rise to dynamically induced symmetry-breaking [50]. This principle can be generalized to ordered phases obstructing other SPT states.

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Supplemental material, available online.

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37. Unlike the intracell interaction $\hat{U} = U \sum_i \hat{\sigma}_i^a \hat{n}_i^b$, $\hat{V}$ is efficient at thermalizing, which is important for dynamically preparing such phases.
38. Our analysis strictly excludes the point $J = 0$, at which the model obeys different symmetries.
39. Supplemental material, available online.
40. While a priori this definition is only valid for translation-invariant systems, corrections for open systems are expected to be sub-leading and can be ignored for large enough system sizes. This is confirmed in our simulations.
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![Figure 5](image)

**Figure 5.** Sketches of the system considered in the main text. Top: system in insulating phase, with half-filling on each sublattice. Bottom: system with orbital ordering of character A (left) and B (right).

**Appendix A: Sketch of System and Phase Diagram Details**

Figure 5 illustrates various phases of the SSH model described by Eq. 1 in the main text. In the non-interacting case, the SSH model is exactly solvable, making it particularly well-suited to study the effects of interaction on edge states, and providing insight into higher-dimensional topology. In the main text, we consider a chain of spinless fermions as the spin degree of freedom adds unnecessary complexity for the physics we wish to elucidate. However, we note that the SSH model can easily be extended to spinful fermions, and the effects we document survive. Moreover its topology is protected by chiral and time-reversal symmetry [52], meaning that it is a class BDI system in the Altland-Zirnbauer classification of random matrices. Thus, the topology should survive in the presence of disorder or weak interactions that preserve these symmetries. Absent interaction, the SSH Hamiltonian can be written in the single-particle basis as

$$\hat{H}_0 = -\sum_j \xi_k \hat{c}_j^\dagger \hat{c}_j \sigma \hat{c}_k$$

where $\xi_k = (\hat{a}_k, \hat{b}_k)$ is a spinor whose components annihilate fermions on sublattice $a$, $b$ respectively with lattice momentum $k$. $\sigma$ denotes the vector of Pauli spin matrices, and

$$\hat{h}_k = (-J - d \cos k, -\tau \sin k, 0), \quad \hat{h}_k^* = 0 \text{ due to chiral symmetry.}$$

Instead of analyzing the single-particle Hamiltonian, we can analyze the SPDM - this provides a natural way of treating mixed states, interacting systems and non-equilibrium scenarios [53].

In the large $V$ limit, the two ground states in the thermodynamic limit have fully occupied (empty) sublattice $a$ ($b$) orbitals, and the particle hole symmetric pair state. Generically, small random fluctuations will drive the system into the symmetry broken state, and the SPT phase is obstructed by spontaneous symmetry breaking. In both the OOBI and OOTI phases, the lowest-order corrections to the ground state are of order $O(\frac{J}{V}, (d + \tau)^2 / V)$, which means that the effect of $J$ survives longer than $d$ or $\tau$, and as $V \to \infty$, we obtain an effective Ising ferromagnet, and we know there are no signatures of topology. Furthermore, the topological character of the system cannot disappear at the onset of the orbital CDW order, as that would imply the existence of a local order parameter for topology. Thus, the transition in the many-body topological invariant must be distinct from the OOBI 2nd-order quantum phase transition.

The breakdown of the single-particle picture can be understood in terms of the relative sizes of the single and many-body gaps. To the left of the green line in the phase diagram Fig. 2 (a), even though the pseudospin gives a winding number of $\mathcal{W} = 1$ for all $V$, the single-particle density matrix becomes increasingly mixed with increasing $V$. This is visualized in Fig. 9, where the radius of the pseudospin covering $\mathbf{r}_k$, (which is still confined to the $xy$-plane) goes to zero, while still encircling the origin as $V \to \infty$. This means that the single particle Hamiltonian remains gapped, but the many-body gap approaches zero. On the other hand, the ordering opens the many-body gap. For large enough $V$, the single-particle gap is irrelevant, and fails to capture the many-body physics.

**Appendix B: Hartree Fock for Weakly Interacting Regime**

For symmetry protected topological (SPT) phases, topological classification tends to be protected from small perturbations that respect the underlying symmetry. In the SSH model considered in the main text, this discussion can be made precise by applying Hartree-Fock theory. When weak interaction (preserving chiral symmetry) is added to the model, the interaction renormalizes the inter-cell hopping strengths, i.e. $H(J, d, \tau, V) \approx H(J, \tilde{d}, \tilde{\tau}, V = 0)$ for new hopping parameters $\tilde{d}$, and $\tilde{\tau}$ in an effective non-interacting model. This subsection details and justifies the application of Hartree-Fock theory to the weakly-interacting model.

The interaction term can be written explicitly in terms of sublattice creation-annihilation operators as

$$\hat{H}_I = V \sum_j \hat{n}_j^a \hat{a}_j^b + \hat{n}_j^a \hat{b}_j^b \quad \text{(A.4)}$$

$$= V \sum_j \hat{a}_j^\dagger \hat{a}_{j+1} \hat{b}_j + \hat{a}_j \hat{b}_{j+1}^\dagger \hat{b}_j^\dagger \hat{b}_j \quad \text{(A.5)}$$

In the Hartree-Fock approximation, the Hamiltonian is approximately transformed back into the non-interacting basis by decoupling the quartic interaction terms into sums of quadratic terms:
FIG. 6. Energy degeneracy computations. (a) and (b) Non-linearly scaled energy difference of lowest lying states, according to 
\[ 1 - \exp(-\Delta E) \].
(a) \( d = 0.0 \); Yellow region near \( J = 0 \) due to finite size effects (b) \( d = 0.4 \); kink in center coincides with crossover from mean-field theory to ordered regime (c) piece-wise linear fit separating singly degenerate (bottom right) from doubly degenerate (upper, left) ground states. Inset: quadratic dependence of slope \( V/J \) of BI-OOBI phase boundary.

\[
\hat{H}_{I,HF} = V \sum_j \left[ \langle \hat{n}_j^a \rangle \hat{n}_{j+1}^b + \langle \hat{n}_j^b \rangle \hat{n}_{j+1}^a \right] \\
+ \langle \hat{n}_j^a \rangle \hat{n}_j^b + \langle \hat{n}_j^b \rangle \hat{n}_j^a + V \sum_j \left[ \langle \hat{a}_j^\dagger \hat{b}_{j+1}^\dagger \rangle \hat{a}_j^\dagger \hat{b}_{j+1} \right] \\
+ \langle \hat{a}_j^\dagger \rangle \hat{b}_{j+1} + \langle \hat{b}_{j+1}^\dagger \rangle \hat{a}_j + h.c., \tag{A.6}
\]

The first summation is the Hartree term, \( \hat{H}_H \), while the second summation is the Fock term, \( \hat{H}_F \).

At half-filling, the system exhibits particle hole symmetry. AB sublattice symmetry ensures that each orbital in the bulk is near half-filling. The interaction we employ preserves particle hole symmetry, so in the presence of weak interaction, this orbital half-filling condition should roughly hold. Thus, we expect that \( \langle \hat{n}_j^{a,b} \rangle \approx \frac{1}{2} \) in the bulk for small \( V \). This means that, in the thermodynamic limit, the Hartree term can be approximated to good accuracy as

\[
\hat{H}_H \approx \frac{V}{2} \sum_j \left[ \hat{n}_j^a + \hat{n}_j^b + \hat{n}_{j+1}^a + \hat{n}_{j+1}^b \right] \approx V \hat{n}_{tot}, \tag{A.7}
\]

Since particle number is conserved, this quantity commutes with the Hamiltonian, and thus just adds a constant shift to the chemical potential.

Moreover, for large systems, we expect the bulk to behave in roughly translationally invariant fashion, so that terms of the form \( \langle \hat{a}_j \hat{b}_{j+1}^\dagger \rangle \) and \( \langle \hat{a}_j^\dagger \hat{b}_{j+1} \rangle \) are approximately independent of site \( j \). This assumption allows us to drastically simplify the Fock term, and as a result the Hamiltonian.

Defining symmetrized and anti-symmetrized combinations of these quantities:

\[
\gamma_{\pm} = \frac{\langle \hat{a}_j \hat{b}_{j+1}^\dagger \rangle \pm \langle \hat{a}_j^\dagger \hat{b}_{j+1} \rangle}{2}, \tag{A.8}
\]

we obtain new effective parameters, \( \bar{d} \) and \( \bar{\tau} \) such that

\[
H(J, \bar{d}, \bar{\tau}, V) \approx H(J, \bar{d}, \bar{\tau}, V = 0).
\]

Namely,

\[
\bar{d} = d + 2V\gamma_+ \tag{A.9}
\]

\[
\bar{\tau} = \tau + 2V\gamma_- \tag{A.10}
\]

FIG. 8. Entanglement gap in symmetry-broken phase as a function of interaction strength for systems of size \( L = 100 \) unit cells, with \( d = 0.4,\, \tau = 1.0 \). (a) Cuts that pass through the Topological Insulating phase (b) and cuts that do not pass through topological phases. Gap opens in (a) when the chiral symmetry is spontaneously broken. In (b), phase transitions are accompanied by non-smooth changes in slope.
In Fig. 7, $\gamma_+\gamma_-$ are computed from DMRG ground-state simulations according to (A.10) for various values of $J$ and $V$, and we explicitly see the weak dependence of $\gamma_+$ on $V$ for fixed $J$. This explains the approximate linearity of the BI $\rightarrow$ TI phase boundary in the weakly interaction regime in Fig. 2 (a) and Fig. 6. Moreover, for $V \leq 3.0$ these simulations show that the variance in $\hat{n}_j^a\hat{n}_{j+1}^a$ and $\hat{n}_j^b\hat{n}_{j+1}^b$ over all sites is less than 1.2% of the mean value for all $J \leq 0.75$. In most cases it is substantially lower, and generically grows as $V$ increases. This means that the translation invariance assumption holds to very good approximation.

### Appendix C: Effective Spin Model for Strongly Interacting Regime

#### Case I: $d = \tau = 0$

As an initial attempt, we disregard topology, setting $d = \tau = 0$, and analyzing the low-energy physics of the resulting model. In this case, we no longer have inter-cell hopping. Our transformation to spin operators takes the form:

$$
\hat{S}_j^z \leftarrow \hat{a}_j^\dagger \hat{a}_j - \hat{b}_j^\dagger \hat{b}_j \quad (A.11)
$$

$$
\hat{S}_j^+ \leftarrow \hat{a}_j^\dagger \hat{b}_j \quad (A.12)
$$

$$
\hat{S}_j^- \leftarrow \hat{b}_j^\dagger \hat{a}_j \quad , \quad (A.13)
$$

We expand $\hat{S}_j^z$:

$$
\hat{S}_j^z \hat{S}_{j+1}^z = (\hat{n}_j^a - \hat{n}_j^b)(\hat{n}_{j+1}^a - \hat{n}_{j+1}^b) \quad , \quad (A.14)
$$

Next, we subtract $\hat{n}_j^a\hat{n}_{j+1}^a$ from both sides. In the strongly interacting regime, translation symmetry in the bulk means that every unit cell has roughly one particle at half-filling. However, we demand even more strongly (a condition which is confirmed to hold true via simulation) $\hat{n}_j^a\hat{n}_{j+1}^a \approx 1$ for all $j$.

Then we can re-express the interaction as:

$$
V \sum_j [\hat{n}_j^b\hat{n}_{j+1}^a + \hat{n}_j^a\hat{n}_{j+1}^b] \approx -\sum_j \frac{1}{2} \hat{S}_j^z \hat{S}_{j+1}^z + \text{const.} \quad , \quad (A.15)
$$

Under this approximation, we can rewrite the Hamiltonian explicitly in terms of spin operators:

$$
\hat{H}_{\text{eff}} = -\sum_j \left[ \frac{2J}{V} \hat{S}_j^x + \hat{S}_j^z \hat{S}_{j+1}^z \right] \quad , \quad (A.16)
$$

and we see that we recover an Ising model in transverse field, with critical field strength dependent on the ratio $J/V$. This explains the approximate linearity of the OOBI $\rightarrow$ OOTI phase boundary in Fig. 2 (a) and Fig. 6. We note that this pseudospin model holds for all values of $J$ and $V$, in the limit that $d = \tau = 0$. In addition, we see that when $V$ dominates (past the critical point), there is a two-fold degeneracy in ground state energy, corresponding to $\otimes_i |\uparrow\rangle_i$ and $\otimes_i |\downarrow\rangle_i$, with all occupation on sublattice $a$ and $b$ respectively. This degeneracy

![FIG. 9. Pseudospin visualizations ($r^z = 0$) for systems of size $L = 100$ unit cells at $d = 0.4$, $J = 0.6$, $\tau = 1.0$ for varying interaction strength. (a) Weak interaction; Still in trivial phase (b) Intermediate interaction strength; Crossover from trivial to topological phase (c) Strong interaction; Single particle picture no longer holds, and $\langle |\mathbf{F}| \rangle \rightarrow 0$ as in Ising ferromagnet.](image)

![FIG. 10. Natural orbital visualizations of single-particle 'edge states' with increasing $V$. $L = 64$ unit cells, at $d = 0.4$, $\tau = 1.0$.](image)
is obviously not related to topology. In addition, while the edge states remain localized for large $V$, we find that their positional expectation values shift inward with increasing $V$, as illustrated in Fig. 10.

Even for $d, \tau \neq 0$, we find that the system behaves like an Ising ferromagnet, with order parameter $\hat{S}_z^2 = \hat{n}_a^2 - \hat{n}_b^2$, as illustrated in Fig. 11. In the strongly interacting phase, without broken symmetry, illustrated in Fig. 10. In the strongly interacting phase, without broken symmetry, $\langle S^z \rangle = 0$ (due to the double degeneracy of the ground state), but the long-range correlations $\langle \hat{S}_a^z \hat{S}_b^z \rangle$ are nonzero. In the symmetry-broken state, obtained by applying positive (negative) on-site energy terms to sublattice a (b) sites, we obtain a nonzero effective magnetization. As a function of interaction strength, $V$, we find the onset of this order to be well-characterized by a second order quantum phase transition of interaction strength, $V$, as illustrated in Fig. 11 (b).

Perturbation Theory Analysis

More formally, we can arrive at a pseudospin model by starting with ground states of the interaction term, and looking at low energy excitations that remain within the eigenspace of the interaction when perturbing $\hat{V}$ with $\hat{H}_0$.

$$|0\rangle_a = \prod_j \hat{a}_j^\dagger |\emptyset\rangle$$
$$|0\rangle_b = \prod_j \hat{b}_j^\dagger |\emptyset\rangle,$$  \hspace{1cm} (A.17)

where $|\emptyset\rangle$ denotes the vacuum. These are the degenerate ground states with all particles in sublattice a (b). These two states have 0 energy with respect to $\hat{V}$.

In the thermodynamic limit, we can ignore boundary effects, and generic first excited states take the form

$$|1\rangle_a = \hat{b}_j^\dagger \hat{a}_{j+1} |0\rangle_a,$$  \hspace{1cm} (A.18)

and similarly for $|1\rangle_b$. These states have energy $E_1 = 1$.

There are multiple ways of generating eigenstates with $E_2 = 1$. Namely, by single application of $\hat{b}_j^\dagger \hat{a}_j$, or terms of the form $\hat{b}_j^\dagger \hat{b}_k^\dagger \hat{a}_j$. Hence, to second order, lowest-lying eigenstates of $\hat{V}$ are given by terms proportional to $J$, and to $(d + \tau)^2$.

We note that in general, other ground states of $\hat{V}$ exist, including states of the form $\prod_j \hat{a}_j^\dagger \hat{b}_j |\emptyset\rangle$ (charge density waves), but the addition of $d$ and $\tau$ favors the ones considered above. We also note that while in the special case $d = \tau = 0$, there is no topology, the model can once again exhibit topological phase transition once $d$ and $\tau$ are added back in.

Appendix D: DMRG Details

For DMRG simulations performed in ITensor, ground states are calculated with maximum truncation error $10^{-8}$, and noise $10^{-10}$ added to the density matrix to facilitate convergence.

To identify the OOBI phase transition points, we compute the ground state averages for orbital charge density wave correlators for a grid of interaction strengths, for system sizes of 48 and 64 sites. The initial guess for critical interaction strength is computed by interpolating an intersection between these two curves. Then, an Adam optimizer is employed to minimize error with all scaled points from both system sizes fitted to one curve. The specific error function used assigns more weight to data near the critical point, reflecting the fact that the scaling should hold more closely as we approach criticality. DMRG yields very good data collapse when treated with the Ising critical exponents. We find that both qualitatively and quantitatively this holds for all $d$. In addition, for different values of $\tau$, the magnitude of the average correlations below and above the critical point change, but the phase transition behavior remains. We note that OOBI behavior does not show up for small systems, and only begins to appear at system sizes of 24 unit cells.

When this quantity is quantized, the topology is well-defined. In strong interaction, it is possible for the Resta polarization to break down [20]. We find that in the interacting
SSH model, the Resta polarization is quantized in all considered regions of parameter-space except for a small region preceding the onset of orbital order. This region is delineated by hatch marks in the phase diagram (Fig. 2(a)). In addition, we note that the boundary between OOBI and OOTI is not exact. While all other phase boundaries were determined with acceptable convergence for systems of size $L = 64$ unit cells, we had to use systems of size up to $L = 140$ unit cells to identify the critical $V$ characterizing the jump in polarization from OOTI to OOBI. Even at this size, we did not see complete convergence in the boundary. However, we can say with confidence that the non-monotonic behavior (dip and rise) in critical $V$ for this transition appears to be a feature in the thermodynamic limit.

In our investigation of charge pumping, we simulated adiabatic evolution by running independent ground state simulations for each pair of parameters $(\Delta, \tau)$ along the cycle, and then smoothly connected this data in post-processing. The specific parameters used in the cycles in Figure 4 are given in Table I. Cycles (a)-(c) were parameterized via

$$\Delta(\theta) = \Delta_0 + R_\Delta \sin(\theta),$$
$$\tau(\theta) = \tau_0 + R_\tau \cos(\theta).$$  \hspace{1cm} (19)$$

whereas cycle (d) was parameterized by

$$\Delta(\theta) = R_\Delta \sin(\theta),$$
$$\tau(\theta) = R_\tau \text{sgn}(\cos(\theta)).$$  \hspace{1cm} (20)$$

| Sub-figure | $J$ | $d$ | $V$ | $\Delta_0$ | $R_\Delta$ | $\tau_0$ | $R_\tau$ |
|------------|-----|-----|-----|------------|------------|----------|----------|
| (a)        | 2.5 | 0.8 | 5.0 | 0.0        | 0.1        | 0.1      | 0.2      |
| (b)        | 0.5 | 0.8 | 3.0 | 0.0        | 0.1        | 0.1      | 0.2      |
| (c)        | 0.2 | 0.4 | 0.3 | 0.001      | 0.0        | 0.0      | 0.5      |
| (d)        | 0.2 | 0.4 | 0.3 | 0.0        | 0.0001     | 0.0      | 0.5      |

TABLE I. Parameter specifications for correlation-assisted charge pumps in Fig. 4