Visualizing topological transport

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We present a mathematically simple procedure for explaining and visualizing the dynamics of quantized transport in topological insulators. The procedure serves to illustrate and clarify the dynamics of topological transport in general, but for the sake of concreteness, it is phrased here in terms of electron transport in a charge-ordered chain, which may be mapped exactly onto transport between edge channels in the Integer Quantum Hall Effect. It has the advantage that it allows a direct visualization of the real-space and real-time evolution of the electronic charges throughout the topological pumping cycle, thus demystifying how charge flows between remote edges separated by an insulating bulk, why the amount of transported charge is given by a topological invariant, and how continuous driving yields a discrete, quantized amount of transported charge.

I. INTRODUCTION

Topology has, over the past decades, taken centre stage alongside symmetry as one of the basic organizing principles of condensed matter physics. As with symmetry, the predictive power associated with topology can be enormous. In the Quantum Hall Effect,\textsuperscript{1} for example, knowing the integer value of a single topological quantum number allows one to predict the transverse conductance of a two-dimensional electron gas with unlimited accuracy, independently of how the electron gas is realised experimentally.\textsuperscript{2,3} Predictions of the transverse conductance have been verified to one part in a billion, and in fact the Quantum Hall Effect now serves as a standard for resistance calibration.\textsuperscript{3} The theoretical understanding of the role of topology underlying the Integer Quantum Hall Effect (IQHE),\textsuperscript{2,3} Fractional Quantum Hall Effect (FQHE),\textsuperscript{5,6} Quantum Spin Hall Effect (QSHE),\textsuperscript{7,8} and more generally Topological Insulators (TIs) and other forms of topological matter,\textsuperscript{9–12} is one of the cornerstones of modern condensed matter physics.\textsuperscript{13,14} Moreover, topological order has been suggested to open the door towards various applications, including dissipationless topological transport, fault-tolerant quantum computation, and the engineering of spin liquid phases of matter.\textsuperscript{13,14}

The typical implication of an insulator being topological, is the presence of conducting states at its edges. The topological nature of these edge states is seen most clearly through the phenomenon of quantized adiabatic particle transport, more commonly known as topological transport or topological pumping.\textsuperscript{15–17} Its idea is easily formulated. By periodically changing some driving force, particles are transferred from one edge of the TI to the opposite side. This transport is quantized, in the sense that for every period of the pumping cycle, precisely an integer number of particles will move between edges.\textsuperscript{15,16} It is topological, because the discrete number of relocated particles is independent of the details of both the system and the driving. As long as the driving is adiabatic, and the system remains insulating, the number of transferred particles will always be the same.\textsuperscript{18} In fact, the topological nature of the pumping can also been seen as an example of the celebrated bulk-boundary correspondence, since the number of particles relayed between opposing edges precisely equals the integer topological quantum number characterising the bulk TI.\textsuperscript{19,20} Topological pumps thus bring together all the main players in the modern understanding of topological matter: quantized conductance, topological quantum numbers, edge states, robustness to perturbations, and the bulk-boundary correspondence.\textsuperscript{21,22} Moreover, the topological pump provides a simple and accessible (thought-)experiment that can be easily introduced even in the early stages of a physics curriculum.

Unfortunately, the intuitive idea of what topological transport entails, is not easily translated into an equally accessible mathematical description of the pumping process in any explicit model.\textsuperscript{22} Here, we remedy this situation by presenting a particular topological pumping process that emphasizes the roles of the key players (the topological invariant, adiabatic pumping, and the connection between opposing edges) and that allows for a straightforward and direct visualization of the particle transport throughout the pumping cycle. The particular model we consider is that of a one-dimensional chain of atoms with electronic charge-order, described at the mean-field level. The analysis of the spectrum, the calculation of a topological invariant, the simulation and visualization of electronic eigenfunctions, and the identification of edge state dynamics are all mathematically accessible in this model. Moreover, the model can be precisely mapped onto the more standard, but more involved, example of topological transport in the IQHE, and it can be straightforwardly generalised to visualize topological transport in other types of TI as well.
II. THE CHARGE-ORDERED CHAIN

As a basic setting for visualizing topological transport, we consider spinless fermions hopping on a one-dimensional lattice, in the presence of nearest-neighbor density-density interactions:

\[
\hat{H} = \sum_{j=0}^{N-1} \left\{ -t \hat{c}_j^\dagger \hat{c}_{j+1} + \frac{V}{2} \hat{c}_j^\dagger \hat{c}_j^\dagger \hat{c}_{j+1} \hat{c}_{j+1} + H.c. \right\}.
\]  

(1)

In this Hamiltonian, the operators \( \hat{c}_j^\dagger \) and \( \hat{c}_j \) respectively create and annihilate a spinless electron at position \( x = ja \), where \( a \) is the lattice constant and \( j \) an integer site label. Notice that for now, we will use periodic boundary conditions, so that the labels \( j \) and \( j + N \) correspond to the same site. The parameter \( t > 0 \) is the amplitude for tunneling of electrons between neighboring sites, and \( V \) is the strength of the nearest-neighbor Coulomb interaction. Weak impurities could be modeled by adding a random on-site potential,\(^{22}\) but we will not consider this aspect here.

As first proposed by Peierls,\(^{23–25}\) and observed in many real and artificial materials,\(^{26–29}\) interacting electrons in a one-dimensional chain are expected to spontaneously organize into a spatially modulated pattern at low temperatures. This so-called charge-density wave (CDW) may be described at the mean-field level by introducing an Ansatz for the local charge density of the form:

\[
\rho(j) = \langle \hat{c}_j^\dagger \hat{c}_j \rangle = \Delta \cos(Qja + \phi). \tag{2}
\]

The CDW amplitude \( \Delta \) serves as an order parameter for the charge-ordered state. The wave number of the CDW is \( Q = n \cdot 2\pi/a \). It is determined by the (fractional) number of electrons per site, or filling fraction \( n = p/q \), with \( p \) and \( q \) co-prime integers. The phase \( \phi \) determines the position of the CDW with respect to the lattice, and varying \( \phi \) corresponds to sliding the charge modulation along the atomic chain.\(^{29}\) In practice, such a sliding motion may be induced in charge-ordered materials by an applied electric field, if it is sufficiently strong to overcome the pinning potential associated with impurities.\(^{30–32}\)

As described in the Supplemental Material, the Ansatz of equation (1) may be used to decouple the interaction term at the mean-field level. After also using the approximation \( \langle \hat{c}_{j-1}^\dagger \hat{c}_{j-1} + \hat{c}_{j+1}^\dagger \hat{c}_{j+1} \rangle \approx 2\rho(j) \), we then find the mean-field CDW Hamiltonian:

\[
\hat{H}_\text{MF} = \sum_{j=0}^{N-1} \left\{ -t(\hat{c}_j^\dagger \hat{c}_{j+1} + \hat{c}_{j+1}^\dagger \hat{c}_j) + 2V \rho(j) \hat{c}_j^\dagger \hat{c}_j \right\}. \tag{3}
\]

Assuming periodic boundary conditions and performing a Fourier transformation, this can be written as:

\[
\hat{H}_\text{MF} = \sum_{0 \leq k < 2\pi/a} \left\{ \frac{1}{2} \epsilon_k \hat{c}_k^\dagger \hat{c}_k + V \Delta e^{i\phi} \hat{c}_k^\dagger \hat{c}_{k+Q} + H.c. \right\}.
\]

Here, \( \epsilon_k = -2t \cos(ka) \) describes the bare band structure. We can conveniently write this Hamiltonian in matrix form:\(^{21}\)

\[
\hat{H}_\text{MF} = \sum_{0 \leq k < 2\pi/a} \left( \begin{array}{ccc} \epsilon_{k+Q} & \Delta & 0 \cdots 0 \Delta^* \\ \Delta^* & \epsilon_{k+2Q} & \Delta & 0 \cdots 0 \\ 0 & \Delta^* & \ddots & \ddots & \vdots \\ \vdots & 0 & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & \Delta & \epsilon_{k+qQ} \end{array} \right). \tag{4}
\]

The parameter \( \Delta \) in this expression equals \( V \Delta e^{i\phi} \), while \( q \) is the denominator in the filling fraction \( n = p/q \), and \( k + qQ = k \) owing to the periodicity of the first Brillouin zone. Note that \( q = 2 \) is a special case, in which the Hamiltonian has a particle-hole symmetry that is absent for all other filling fractions, and we will not consider it here.

III. COMPARISON TO THE IQHE

Numerical diagonalisation of \( H_k \) yields the energy spectrum, or band structure, for any given value of the CDW phase \( \phi \), as shown in figure 1A. Collecting the energy bands associated with all possible choices for \( k \) and \( \phi \), for a given filling fraction \( n = p/q \), and plotting them as dots in the plane of energy versus filling fraction, yields a version of the famous Hofstadter butterfly spectrum,\(^{21,33,34}\) shown in figure 1B. For the specific case \( \Delta = t \), equation (4) becomes equivalent to the matrix form of Harper’s equation, applied by Hofstadter to model the IQHE in a two-dimensional electron gas subjected to a strong magnetic field.\(^{33}\) We thus find that the physics of sliding CDW may be mapped onto that of the IQHE.\(^{21,34}\) The filling fraction of the charge-ordered system, and hence its CDW periodicity, then correspond to the magnetic field strength perpendicular to the surface of a quantum Hall cylinder, which determines the filling of its Landau levels.\(^{21,33,35}\) Under the same mapping, the phase \( \phi \) of the CDW order parameter translates to a flux threading the quantum Hall cylinder,\(^{20}\) while the spatial coordinate of the CDW chain is directly related to the spatial coordinate parallel to the axis of the IQHE cylinder. The mapping is indicated schematically in figure 1C.

In the semi-classical picture of the IQHE, electrons in a two-dimensional electron gas are confined to cyclotron orbits that are much smaller than the spatial extent of the system. If the electron gas is confined to the surface of a torus (periodic boundary conditions in all directions),
Given filling fraction.

Appendix A how to calculate the topological invariant spectrum of the periodic chain.

16, 21, 22, 34

which is a single integer number characterising the bulk determined in terms of a so-called topological invariant, of the edge state conductance in an open chain may be the ends of the chain appear. As in the IQHE, the value with open boundaries, edge states that are localised at conditions are applied. When we consider a finite chain the case takes place along the edges of the system, is charge transport will be possible. The conductance in

\[ \langle \hat{c}_j^\dagger \hat{c}_j \rangle \]

\[ (c_j^\dagger c_j) \]

\[ j = 0, 1 \ldots \]

\[ \frac{2\pi - \phi}{Q}, \frac{2\pi}{Q} \]

The dispersion relation for the mean-field CDW with periodic boundary conditions. Different colors correspond to different values of \( \phi \), ranging between zero and \( 2\pi \).

**B** The spectrum of the mean-field CDW as a function of filling fraction. For each \( n \), ranges are indicated for all energy eigenvalues found as \( ka \) is varied between \( -\pi/(3a) \) and \( \pi/(3a) \), and \( \phi \) is varied between zero and \( 2\pi \). The resulting figure is known as Hofstadter’s butterfly, and was first found in a tight-binding model for the IQHE.

To create dispersion relation, we considered 50 \( k \)-points, and used the (arbitrary) parameter values \( U = t, \Delta = 0.5t \), and \( Q = 2\pi/(3a) \). The phase \( \phi \) was varied between zero and \( 2\pi \) in ten steps. The Hofstadter butterfly contains all fractions \( n = p/q \) with \( p \) and \( q \) co-prime integers and \( q \) ten or less. For each the spectrum was calculated for 200 steps in both \( k \) and \( \phi \).

IV. TOPOLOGICAL TRANSPORT

The real-space Hamiltonian describing a one-dimensional, charge-ordered chain with \( N \) sites can be written as:

\[ \hat{H}_{MF} = (c_{j=0}^\dagger c_{j=1} c_{N-1}^\dagger) h \]

\[ \begin{pmatrix} \hat{c}_0 \\ \hat{c}_1 \\ \vdots \\ \hat{c}_{N-1} \end{pmatrix} \]

\[ \begin{pmatrix} \epsilon_0 & -t & 0 & \ldots & 0 & -\tilde{t} \\ -t & \epsilon_1 & -t & \ldots & 0 \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ 0 & 0 & \ldots & \tilde{t} & \epsilon_{N-1} \end{pmatrix} \]

Here, we defined \( \epsilon_j = 2V\Delta \cos(Qja + \phi) \), and we again use the approximation \( \langle \hat{c}_j^\dagger \hat{c}_{j+1} \rangle \approx 2\rho(j) \), independent of the boundary conditions. The elements \( \tilde{t} \) at the corners of the matrix can then be used to model different types of connections between the edges of the system.

Although it is one of the central manifestations of topology, the fact that the quantisation of charge transport between the edges of a finite system is determined by an integer number characterising a different system without edges, may well seem counterintuitive. It may become even more so once you realise that the topological invariant may be negative as well as positive. In the 1/3-filled CDW, for example, a single electron is transported every pumping cycle in the direction of sliding, but a 2/3-filled CDW instead transfers an electron in the direction opposite to the sliding. Several more counterintuitive questions naturally arise, including how the electrons cross between edges of the CDW chain, even though the bulk is strictly insulating and the macroscopic distance between the edges suppresses any direct tunneling; or what the amount of charge localised on each edge is, at any given moment during the pumping cycle. To give a clear and intuitive answer to these questions, we will visualize the topological pumping process in the finite CDW chain in real space and real time.
chain. The periodic boundary conditions considered before correspond to \( \tilde{t} = t \). Having an open chain with nothing attached to the edges, is given by \( \tilde{t} = 0 \). An intermediate case, where the edges are connected via a weak link, corresponding for example to an additional wire in an experimental implementation, may be modeled by taking \( 0 < \tilde{t} \ll t \).

Taking open boundary conditions, the matrix of equation (5) may be diagonalised numerically for moderate values of \( N \). For each value of the phase \( \phi \), there are \( N \) different eigenvalues, as shown in figure 2. For the system with periodic boundary conditions, these would correspond to eigenvalues with distinct momentum values. Taking open boundary conditions, they instead become standing waves, with nodes at the edges of the chain, and various numbers of zeroes in between. These can be visualized directly by plotting the eigenvectors of \( h \), and as shown in figure 2 they indeed look like particle-in-a-box states, modulated by the periodic CDW.

For certain special values of \( \phi \) we also find energy eigenvalues inside what would have been the band gap for the periodic chain. The corresponding eigenvectors reveal these special states to be exponentially localised at either the right or left edge of the open chain. Two edge states, one localised on the right, and one on the left, cross each other in energy as \( \phi \) is varied. The states can be degenerate there, because their exponential localisation results in zero wave function overlap between them.

Once we add a connection between the edges, taking \( \tilde{t} \) to be small but non-zero, the degeneracy will be lifted, as shown in figure 3B.

To visualize the topological transport, we now consider for example the 1/3-filled CDW of figure 3A in its ground state with \( \phi = 0 \). All bulk states in the lowest band are then occupied, and all higher bands are empty. Adiabatically varying \( \phi \) implies driving it slowly enough for each eigenstate to not change its occupation. As \( \phi \) grows, the states in the lowest band thus remain occupied. As \( \phi \) becomes greater than approximately \( \pi/3 \), one of the bulk bands is slowly transformed into a state localised at the left edge of the CDW chain. Since we vary \( \phi \) adiabatically however, it remains occupied. In fact, for \( \tilde{t} = 0 \), we can continue adiabatically to \( \phi \gtrsim 2\pi/3 \), and find the occupied left edge state entering the bulk of the second band, while the topmost state of the first band has become unoccupied. After a full cycle, at \( \phi = 2\pi \),
the system is in an excited state, with an electron state occupied in the second band, and a hole present in the first.

Although energy is pumped into the system, this is not yet the quantized electron pump we were hoping for. To usefully employ a device that pumps electrons from one of its edges to another, you need to connect the edges by a wire, and use the flow of electrons to do work. Such an external connection between the edges can be modelled in the Hamiltonian of equation (5) by taking $t$ to be small, but non-zero. A small gap between the crossing edge states then opens up, as shown in figure 3B, and under adiabatic variation of $\phi$ the highest bulk state in the first band becomes a left edge state at $\phi \approx \pi/3$, then crosses through the external wire as the edge states undergo an avoided crossing, and comes back at the right edge of the CDW chain for $\phi \approx 2\pi/3$. After a full cycle, the system is back in its initial state, and ready to be used again.

During the cycle, a single electron is adiabatically pumped from a left CDW edge state to the right, allowing the extraction of work. The entire evolution of the electronic wave function can be followed and visualized as a function of time, as shown in figure 3C. The fact that precisely a single electron is transferred, is due to there being one set of single-electron edge states crossing the first band gap. For a 2/3-filled CDW chain, three electrons will flow through the wire. Since the two electrons in the first band gap flow in opposite directions, they do not contribute to the overall transport. The single electron transferred between edge states in the second band gap flows from right to left, and thus constitutes a current in the direction opposite to the sliding motion of the CDW.

V. DISCUSSION

The fact that the discrete number of particles pumped during a topological transport cycle coincides with the Chern number can now be given an intuitive interpretation. Both of them arise from a single phenomenon, namely the inversion of bands in the energy spectrum. Starting from the 2/3-filled, one-dimensional chain with $\Delta = 0$, the second, occupied band touches the third, unoccupied band at one point, $k = 0$. Even if $\Delta$ is non-zero, the occupied state just left of $k = 0$ will differ qualitatively from that just to the right, since it originates from a different band. The Chern number can be thought of as effectively keeping count of the number of such so-called band inversions. In a system with open boundaries, these same inverted states cannot smoothly connect to the vacuum, and become exponentially localised at the edge.

If the system is large, so that edge state wave functions do not overlap, they will cross and become degenerate in the band gap. These crossings are exploited during topological transport to adiabatically transfer a discrete number of charges from one side of the system to the other. Visualizing this process by directly plotting the wave functions of an accessible model system in real space and real time clarifies the nature of the topological transport, and gives an intuitive understanding for why the transport is quantized, why it requires a non-zero topological invariant, and what happens to the electronic wave function of the transported charges throughout the pumping cycle.

The one-dimensional CDW system discussed here has the advantage that it allows a direct visualization of the topological transport. The conclusions, however, are not unique for this system. As we saw before, the mean-field CDW Hamiltonian can be mapped onto a strong-coupling model for the IQHE on a two-dimensional cylinder. The electronic states in the IQHE setup are less straightforward to visualize and follow in time, both because of their two-dimensional nature, and because of the minimal coupling between momentum and magnetic flux in the gauge-independent canonical momentum. The spectrum of states for the IQHE, however, is the same as that of figures 1 and 2, with the caveat that $\phi$ now labels canonical momentum and all states in the lowest band, for all values of $\phi$, are simultaneously occupied. Laughlin’s gauge argument then shows that under the insertion of an additional flux quantum in the IQHE cylinder, all states increase their momentum value by one unit, moving one step in the diagram of figure 2. It is straightforwardly checked that the effect is the same as that of the topological pump discussed here in the CDW context. That is, for $n = 1/3$, a single electron moves from being localised along the perimeter at the left end of the cylinder, to the right.

The visualization of topological transport established here for a particularly accessible example system, can be directly adopted for models of the Integer Quantum Hall Effect, the Quantum Spin Hall Effect, and gives qualitative insight into the emergence of edge states and quantized adiabatic particle transport in all types of topological insulators.

Appendix A: Calculating the topological invariant

Using for example the Kubo formula, the Hall conductance of a two-dimensional electronic system with periodic boundary conditions may be written as:

$$\sigma_H = \frac{e^2}{h} \sum_{m \in \text{occ}} c_m \sum_{m \in \text{occ}} c_m$$

$$c_m = \frac{-i}{2\pi} \int d\vec{k} \int d\vec{x} \left( \partial_{\vec{x}} \psi^m_{k}(\vec{x}) \right)^\ast \left( \partial_{\vec{x}} \psi^m_{k}(\vec{x}) \right) - \text{c.c.}$$

Here, the spatial integral runs over one unit cell, while the momentum integrals cover the first Brillouin zone. The index $m$ labels bands in the band structure, and is summed over occupied bands only. The wave function $\psi^m_{k}(\vec{x})$ is the $m$th eigenfunction of the Bloch Hamiltonian $H_k$. The integrand in the final line is known as the Berry
curvature for the completely occupied band \( m \), and the number \( c_m \) as its Chern number. As we will see, the contribution \( c_m \) of band \( m \) to the conductivity does not depend on the energies of the states in the band, and \( c_m \) is therefore a topological invariant that is unaffected by any deformations of the Hamiltonian that do not cause bands to cross.

To evaluate \( c_m \) for the bands in the model of equation (4), we interpret \( k \) and \( \phi \) to correspond to the \( k_x \) and \( k_y \) coordinates in equation (A1). It may then seem like we need to explicitly need to find the wave functions \( \psi_k^\alpha(x) \). In fact, however, the only thing that matters is how the wave function changes as one goes around the Brillouin zone, not what it is for any particular momentum. To see the evolution of the wave function as a function of \( k \) and \( \phi \) it suffices to find the wave function at some selected points in the Brillouin zone, and then interpolate smoothly between those.

For concreteness, consider filling fraction \( n = 1/3 \), so that there are three bands in the spectrum, with one band occupied. First consider the non-interacting model with \( \Delta = 0 \). The Hamiltonian \( H_k \) is then diagonal, and the bands correspond to electrons created by \( \hat{c}_k \) and \( \hat{c}_k^\dagger \). For non-zero \( \Delta \) the eigenstates will instead become superpositions of these three contributions, of the form \( A \hat{c}_{k+Q}^\dagger + B \hat{c}_{k+2Q}^\dagger + C \hat{c}_k^\dagger \). Focusing first on lowest, occupied band at the point \( k = 0 \), we know that at \( \Delta = 0 \) and for any value of \( \phi \), it corresponds to the state with \( A = B = 0 \) and \( C = 1 \). For small, but non-zero \( \Delta \), the coefficients \( A \) and \( B \) become of order \( \Delta/E \), where \( E \) is the energy separating the lowest band from the higher two bands. Since \( E \) is large, we may approximate the lowest band at \( k = 0 \) to correspond purely to \( \hat{c}_k^\dagger \). As will become clear shortly, the small error in assigning this wave function at this point will not affect the value of the Chern number at all.

Following the same line of reasoning, we can consider the state at \( k = -\pi/(3a) \), again for any value of \( \phi \). Here, the lowest two bands are degenerate, and will both contribute to the wave function for non-zero \( \Delta \). The highest band, however, is again well-separated from the others in energy, and may be ignored to first order in \( \Delta/E \). To find the wave function of the lowest energy state, we thus consider only the rows and columns of \( H_k \) associated with \( \hat{c}_k^\dagger \) and \( \hat{c}_{k+Q}^\dagger \). This yields a 2x2 matrix that can be straightforwardly diagonalised, giving a lowest energy state with \( A = -e^{-i\phi}\sqrt{1/2} \), \( B = 0 \), and \( C = \sqrt{1/2} \). Repeating the same arguments at \( k = \pi/(3a) \) gives a wave function there with \( A = 0 \), \( B = -e^{i\phi}\sqrt{1/2} \), and \( C = \sqrt{1/2} \).

It now turns out to be impossible to define smooth functions \( A(k,\phi) = \hat{A}(k)e^{-i\phi} \), \( B(k,\phi) = \hat{B}(k)e^{i\phi} \), and \( C(k,\phi) = \hat{C}(k) \) that reduce to the obtained values for \( A, B, \) and \( C \) at the three \( k \)-points spanning the Brillouin zone. What is possible, however, is to divide the Brillouin zone into two regions, \( k \in [-\pi/(3a),0] \) and \( k \in [0,\pi/(3a)] \), and find two sets of functions that interpolate smoothly between the end points for each region individually. The topological nature of the Chern number then becomes immediately apparent when we write equation (A1) in terms of the interpolating functions:

\[
c_1 = \frac{-i}{2\pi} \int_0^{2\pi} d\phi \left[ -2i \int_{-\pi/(3a)}^0 dk \frac{\partial \hat{A}(k)}{\partial k} \tilde{A}(k) + 2i \int_0^{\pi/(3a)} dk \frac{\partial \hat{B}(k)}{\partial k} \tilde{B}(k) \right]
\]

\[
= -\frac{1}{\pi} \int_0^{2\pi} d\phi \left[ \int_{\hat{A}(0)}^{\hat{A}(\pi/(3a))} \hat{A} \hat{d} \hat{A} - \int_{\hat{B}(0)}^{\hat{B}(\pi/(3a))} \hat{B} \hat{d} \hat{B} \right]
\]

\[
= 1.
\]

Notice that we could evaluate the integrals without ever specifying the precise form of the functions \( \hat{A}(k) \) and \( \hat{B}(k) \). This shows what it means for the Chern number to be topological: we can span the wave function in the Brillouin zone from its values at the points where a gap has been created, and the Chern number is completely insensitive to how we interpolate between these end points. We can thus freely deform the Hamiltonian, and change the interpolating function. As long as the deformations do not close the gap at the Fermi level, and necessitate mixing of occupied and unoccupied states, the value of \( c_1 \) remains unaffected.

A similar calculation will show that the Chern number \( c_2 \) for the second band equals \(-2 \), while that for the uppermost band is again \(1 \). In terms of quantized transport between edges in an open CDW chain, this means that for filling fraction \( n = 1/3 \) sliding the CDW over a single wave length results in a single electron being transferred in the direction of sliding. For a filling of \( n = 2/3 \) we have \( c_1 + c_2 = -1 \), so that a single electron will instead be transferred in the direction opposite to the sliding motion.

**Appendix B: Supplementary Material**

In this supplementary material, we present the detailed steps involved in the calculations of the main text. We hope these may serve as a convenient starting point for formulating exercises, questions, and simulations connected to the visualization of topological transport.

1. **The mean-field Hamiltonian**

To find the mean-field description of the charge-ordered chain, we start from the Hamiltonian:

\[
\hat{H} = \sum_{j=0}^{N-1} \left\{ -t \hat{c}^\dagger_j \hat{c}_{j+1} + \frac{V}{2} \hat{c}^\dagger_j \hat{c}_j \hat{c}^\dagger_{j+1} \hat{c}_{j+1} + \text{H.c.} \right\}.
\]

Here, H.c. denotes the Hermitian conjugate. Recall that the operators \( \hat{c}^\dagger_j \) and \( \hat{c}_j \) respectively create and annihilate
a spinless electron at position \( x = ja \), where \( a \) is the lattice constant and \( j \) an integer site label. Notice that for now, we will use periodic boundary conditions, so that the labels \( j \) and \( j + N \) correspond to the same site. The parameter \( t > 0 \) is the amplitude for tunneling of electrons between neighbouring sites, and \( V \) is the strength of the nearest-neighbor Coulomb interaction.

The idea behind the mean-field analysis, is that we expect to be able to make a reasonable guess for the ground state expectation value of the electron density \( \rho(j) \equiv \langle \hat{c}_j^\dagger \hat{c}_j \rangle \). At the end of the calculation, one may check that the initial guess is indeed consistent with the mean-field model we end up with. To see how we can use the fact that we know what to expect for the density operator, first rewrite it as:

\[
\hat{c}_j^\dagger \hat{c}_j = \langle \hat{c}_j^\dagger \hat{c}_j \rangle + \hat{f}_j
\]

with \( \hat{f}_j \equiv \hat{c}_j^\dagger \hat{c}_j - \langle \hat{c}_j^\dagger \hat{c}_j \rangle \). (B2)

This expression defines the fluctuation operator \( \hat{f}_j \), and does not involve any approximation yet. Assuming that we do have a good Ansatz for the expectation value of the electron density however, we may assume that the expectation value of the fluctuations \( \hat{f}_j \) is small, and its square even smaller. We can use this by rewriting the Hamiltonian in terms of the fluctuation operator, and then neglecting all terms of quadratic (or higher) order in the fluctuations:

\[
\hat{H} \approx \sum_{j=0}^{N-1} \left\{ -t \langle \hat{c}_j^\dagger \hat{c}_{j+1} + \hat{c}_{j+1}^\dagger \hat{c}_j \rangle \\
+ V \left( \langle \hat{c}_j^\dagger \hat{c}_j \rangle + \hat{f}_j \right) \left( \langle \hat{c}_{j+1}^\dagger \hat{c}_{j+1} \rangle + \hat{f}_{j+1} \right) \right\}
\]

\[
\approx \sum_{j=0}^{N-1} \left\{ -t \langle \hat{c}_j^\dagger \hat{c}_{j+1} + \hat{c}_{j+1}^\dagger \hat{c}_j \rangle \\
+ V \langle \hat{c}_j^\dagger \hat{c}_j \rangle \hat{f}_{j+1} + \langle \hat{c}_{j+1}^\dagger \hat{c}_{j+1} \rangle \hat{f}_j \\
+ \langle \hat{c}_j^\dagger \hat{c}_j \rangle \langle \hat{c}_{j+1}^\dagger \hat{c}_{j+1} \rangle \right\}
\]

(B3)

In the final line, we can use equation (B2) to write the remaining fluctuation operators in terms of density operators again, and then replace the expectation values \( \langle \hat{c}_j^\dagger \hat{c}_j \rangle \) with the Ansatz \( \rho(j) \) for the electron density.

\[
\hat{H} \approx \sum_{j=0}^{N-1} \left\{ -t \langle \hat{c}_j^\dagger \hat{c}_{j+1} + \hat{c}_{j+1}^\dagger \hat{c}_j \rangle \\
+ V \left( \rho(j) \hat{c}_{j+1}^\dagger \hat{c}_j + \rho(j+1) \hat{c}_j^\dagger \hat{c}_{j+1} \\
- \rho(j) \rho(j+1) \right) \right\}
\]

\[
= \sum_{j=0}^{N-1} \left\{ -t \langle \hat{c}_j^\dagger \hat{c}_{j+1} + \hat{c}_{j+1}^\dagger \hat{c}_j \rangle \\
+ V \left( \rho(j-1) + \rho(j+1) \right) \hat{c}_j^\dagger \hat{c}_j \\
- 2V \rho(j) \rho(j+1) \right\}.
\]

(B4)

In the second line, we used the periodic boundary conditions to shift the summation index in one of the terms. The final term in this Hamiltonian, \(-2V \rho(j) \rho(j+1)\) is a constant that can be absorbed into a suitable redefinition of the zero of energy. Since the charge density is a smooth and continuous function of space, we can also use the approximation \(\langle \hat{c}_j^\dagger \hat{c}_{j-1} + \hat{c}_{j+1}^\dagger \hat{c}_{j+1} \rangle \approx 2 \rho(j)\), to find the final form of the mean-field CDW Hamiltonian:

\[
\hat{H} \approx \sum_{j=0}^{N-1} \left\{ -t (\hat{c}_j^\dagger \hat{c}_{j+1} + \hat{c}_{j+1}^\dagger \hat{c}_j) \\
+ 2V \rho(j) \hat{c}_j^\dagger \hat{c}_j \right\}
\]

= \hat{H}_{\text{MF}}. \quad \text{(B5)}

In this mean-field Hamiltonian, we can finally make the assumption \( \rho(j) = \Delta \cos(Qja + \phi) \), with \( \Delta \) the CDW amplitude, \( Q \) the CDW wave number, and \( \phi \) its phase. Finding and minimizing the ground state energy, in principle allows us to check that the mean-field Ansatz is self-consistent. Since this is not essential for the CDW topology, we will not elaborate on the self-consistency conditions here.

2. Alternative boundary conditions

Notice that the mean-field Hamiltonian of equation (B5) can immediately be put into matrix form:

\[
\hat{H}_{\text{MF}} = \left( \begin{array}{cccc}
\hat{c}_0 \\
\hat{c}_1 \\
\vdots \\
\hat{c}_{N-1}
\end{array} \right)^\dagger \left( \begin{array}{cccc}
\epsilon_0 & -t & 0 & \ldots & 0 \\
-t & \epsilon_1 & -t & \ldots & 0 \\
0 & -t & \ddots & \ddots & \vdots \\
\vdots & 0 & \ddots & \ddots & 0 \\
0 & \ldots & -t & 0 & \epsilon_{N-1}
\end{array} \right) \left( \begin{array}{c}
\hat{c}_0 \\
\hat{c}_1 \\
\vdots \\
\hat{c}_{N-1}
\end{array} \right),
\]

\quad \text{(B6)}

Here, we defined \( \epsilon_j = 2V \rho(j) = 2V \Delta \cos(Qja + \phi) \). The elements \( t \) at the corners of the matrix are equal to \( t \) for the periodic boundary conditions studied so far. They can also be used to implement different boundary conditions. Having an open chain with nothing attached to the edges, for example, is described by using \( t = 0 \). An intermediate case, where the edges are connected via a weak link, corresponding for example to an additional wire in an experimental implementation, may be modeled by taking \( 0 < t \ll t \).
3. The Fourier-transformed Hamiltonian

Assuming periodic boundary conditions again, we can introduce Fourier-transformed operators by defining:

\[ \hat{c}^\dagger_k = \sqrt{1/N} \sum_{j=0}^{N-1} e^{-i k j a} \hat{c}^\dagger_j \]

\[ \hat{c}_k = \sqrt{1/N} \sum_{j=0}^{N-1} e^{i k j a} \hat{c}_j. \]  

(B7)

Here, the variable \( k \) signifies the (crystal) momentum of electrons in momentum eigenstates created by \( \hat{c}^\dagger_k \). Because of the finite length of the periodic real-space lattice, the allowed values of the crystal momentum \( k \) are discrete. The discrete nature of the real-space lattice at the same time guarantees the momentum states to be periodic. For the one-dimensional chain then, \( k \) can have discrete values \( 2\pi m/(Na) \), with \( m \in \{0, 1, 2, \ldots, N-1\} \).

Periodicity of \( k \) means in this context that \( \hat{c}^\dagger_k \) creates the same electronic state as \( \hat{c}^\dagger_{k+2\pi/a} \). The inverse transformations expressing real-space operators in terms of momentum-space ones, are given by:

\[ \hat{c}^\dagger_j = \sqrt{1/N} \sum_{0 \leq k < 2\pi/a} e^{i k j a} \hat{c}^\dagger_k \]

\[ \hat{c}_j = \sqrt{1/N} \sum_{0 \leq k < 2\pi/a} e^{-i k j a} \hat{c}_k. \]

(B8)

These definitions can be substituted directly into the Hamiltonian of equation (B5):

\[ \hat{H}_{MF} = \frac{1}{N} \sum_k \sum_{k'} \left[ -t e^{i k j a} e^{-i k' j a} - t e^{i (k+1) j a} e^{-i k' j a} + 2 V \Delta \cos(Q j a + \phi) e^{i k j a} e^{-i k' j a} \right] \hat{c}^\dagger_k \hat{c}_{k'}. \]  

(B9)

In these expressions, we can write the cosine as a sum of exponentials:

\[ 2 \cos(Q j a + \phi) = e^{i(Q j a + \phi)} + e^{-i(Q j a + \phi)}. \]  

(B10)

Substituting the definition of the delta function \( \delta_{k,k'} = 1/N \sum_j e^{i(k-k') j a} \), then allows us to perform the sum over one of the momenta:

\[ \hat{H}_{MF} = \frac{1}{N} \sum_k \sum_{k'} \left\{ -t \delta_{k,k'} e^{-i k' a} - t \delta_{k,k'} e^{i k a} + V \Delta e^{i \phi} \delta_{k+Q,k'} + V \Delta e^{-i \phi} \delta_{k+Q,k} \right\} \hat{c}_{k}^\dagger \hat{c}_{k'} \]

\[ = \sum_{0 \leq k < 2\pi/a} \left\{ -2 t \cos(k a) \hat{c}_{k}^\dagger \hat{c}_{k} + V \Delta e^{i \phi} \hat{c}_{k+Q}^\dagger \hat{c}_{k} + V \Delta e^{-i \phi} \hat{c}_{k}^\dagger \hat{c}_{k-Q} \right\}. \]  

(B11)

This is the same form for the Fourier transformed Hamiltonian as that used in the main text.

4. Writing the Hamiltonian in matrix form

To facilitate the use of numerical software for calculating the eigenvalues of the Hamiltonian, it is convenient to write it in matrix form. We would thus like to find an expression of the form:

\[ \hat{H}_{MF} = \sum_k \begin{pmatrix} \hat{c}_{k+Q}^\dagger \hat{c}_{k+Q} & \hat{c}_{k+2Q}^\dagger \hat{c}_{k+2Q} & \cdots & \hat{c}_{k+NQ}^\dagger \hat{c}_{k+NQ} \end{pmatrix} H_k \begin{pmatrix} \hat{c}_k+Q \\ \hat{c}_{k+2Q} \\ \vdots \\ \hat{c}_{k+NQ} \end{pmatrix}. \]

In this expression, we assumed \( Q = n \cdot 2\pi/a \), with \( n = p/q \) a co-prime fraction, so that periodic boundary conditions imply \( \hat{c}_{k+qQ}^\dagger = \hat{c}_k^\dagger \). Writing the Hamiltonian this way, however, one should be careful about the values \( k \) is summed over. If we simply sum over the values \( 2\pi m/(Na) \), with \( m \in \{0, 1, 2, \ldots, N-1\} \), electrons with momentum equal to for example \( 3Q/2 \) will be created both by the first component \( \hat{c}_{k+Q}^\dagger \) of the vector of creation operators (for \( k = Q/2 \)), and by the final component \( \hat{c}_{k+qQ}^\dagger \) in the vector (for \( k = 3Q/2 \)). Since it would be convenient for the vector of creation operators to describe an orthonormal basis for the Hamiltonian matrix \( H_k \), so that its eigenvalues directly correspond to the energies defined by \( \hat{H}_{MF} \), it is preferable to avoid electronic states appearing in multiple components. This can be achieved by restricting the range of momentum values summed over to \( 2\pi m/(Na) \), with \( m \in \{0, 1, 2, \ldots, N/q-1\} \). To find the matrix \( H_k \) then, we first rewrite the equation for \( \hat{H}_{MF} \) such that it contains only a sum over this restricted range of momentum values:

\[ \hat{H}_{MF} = \sum_{0 \leq k < 2\pi/a} \left\{ c_{k+Q}^\dagger c_{k+Q} + V \Delta e^{i \phi} c_{k+Q}^\dagger c_{k+Q} + V \Delta e^{-i \phi} c_{k}^\dagger c_{k-Q} \right\}. \]  

(B12)
Writing out this equation in the desired matrix form, yields the final expression for $H_k$:

$$H_k = \begin{pmatrix}
\epsilon_{k+Q} & \Delta & 0 & \ldots & 0 & \Delta^* \\
\Delta^* & \epsilon_{k+2Q} & \Delta & 0 & \ldots & 0 \\
0 & \Delta^* & \ddots & \ddots & \vdots \\
\vdots & 0 & \ddots & \ddots & \ddots \\
0 & \vdots & \ddots & \ddots & \ddots \\
\Delta & 0 & \ldots & 0 & \Delta^* & \epsilon_{k+qQ}
\end{pmatrix}. \quad (B13)$$

Recall that here, $\Delta = V\Delta e^{i\phi}$, and $k + qQ = k$ owing to the periodicity of the first Brillouin zone. Note that this form of the matrix does not apply to the special case $q = 2$, which we do not consider.

5. Suggested exercises

- Reproduce the derivations in sections B1-B4 above.
- Make an animation of the topological transport in

the mean-field CDW chain. That is, plot the wavefunction $|\psi_j|^2$ of the occupied state with the highest energy in figure 3 of the main text, for some initial value of the phase $\phi$. Then animate cyclic variations of $\phi$. Do this for different values of the model parameters (in particular $i/t$).

- (more advanced) Include weak impurities in the model by adding a potential energy $\sum_j \eta(j)$ to the Hamiltonian, where for every $j$, $\eta(j)$ is an independent random number between $-t/5$ and $t/5$. Observe the effect of the impurities on eigenfunctions in the bulk (they typically become more localised), while the topological transport is unaffected (the quantized transport still occurs).

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Notice that the restricted range of momenta consists precisely of all momenta within the reduced Brillouin zone that corresponds to the enlarged real-space unit cell of size $qa$ in the CDW state.