Visualizing topological transport in charge ordered materials

Mariya A Lizunova$^{1,2}$, Cristiane Morais Smith$^1$, Jasper van Wezel$^2$

$^1$Utrecht University - Princetonplein 5, 3584 CC Utrecht, The Netherlands
$^2$University of Amsterdam - Science Park 904, 1098 XH Amsterdam, The Netherlands

E-mail: vanwezel@uva.nl

Abstract. Electron pumping in topological materials has attracted a lot of attention recently. Even in the most intensely studied example, the integer quantum Hall cylinder, the detailed dynamics of topological charge transport remains difficult to visualize, due to the presence of gauge symmetry. Here, we exploit the absence of gauge freedom in one-dimensional charge ordered systems subject to an external driving force, to demonstrate details of their topological pumping. Inspection of the instantaneous eigenstates of a particular mean-field charge ordered model reveals an interplay between topological edge states and the mobility edge. The results also allow us to visualize adiabatic (Thouless) pumping in general charge ordered materials and other topological systems.

1. Introduction

The integer quantum Hall effect (IQHE) [1] arises in two-dimensional (2D) electron gas in a strong perpendicular magnetic field, and is characterized by an insulating bulk, combined with metallic edges. Building on analogies with the IQHE, there is unabated interest in identifying new types of topological materials [2, 3, 4, 5, 6, 7], for which new topological invariants (such as various types of Chern numbers or spin-Chern numbers) were identified [8]. These systems have edge currents that are quantized and protected by symmetries of the system, which have been suggested to be useful for applications in quantum nanotechnology [6, 7].

The Harper’s equation [9, 10] defining the IQHE in 2D also provides a mean-field description of sliding commensurate charge-density waves (CDW) in one-dimensional (1D) [11, 12]. An effectively 2D Brillouin zone (BZ) can constructed for the CDW by combining the momentum ($k$) with the phase ($\phi$) of the complex order parameter in the CDW model. Upon varying $\phi$ adiabatically from 0 to $2\pi$, the CDW slides over precisely one wavelength. The Hamiltonian for the sliding 1D CDW [12] and for the 2D IQHE [13] may be mapped onto each other by identifying $k$ with $k_x$ and $\phi$ with $k_y$. The mapping also relates the quantized adiabatic transport (Thouless pump) in charge ordered systems to the topological transport between edge states upon insertion of a flux quantum in a quantum Hall cylinder (Laughlin’s gauge argument) [8, 14, 15]. The latter is caused by adiabatically threading an Aharonov-Bohm flux quantum $\phi_0 = h/e$ through an IQHE cylinder [16]. Electrons then move from one edge of the cylinder to another, and the number of transported electrons is precisely defined by the Chern number of the occupied states in the 2D BZ [17].

Despite intense investigation [18, 19, 20, 21], and some recent experimental progress [22, 23, 24], the detailed dynamics of topological charge transport remains difficult to visualize due to
the presence of gauge freedom associated with the electromagnetic vector potential in the IQHE setup [25, 26]. Here, we use the absence of gauge freedom in CDW systems to realize something new: to get a detailed picture of the real-time topological transport as electrons flow from one edge to the other.

Our strategy is the following. First, we introduce a tight-binding model, and account for nearest-neighbor interaction within a mean-field approximation. Plotting the numerically obtained instantaneous eigenstates at different stages of the topological transport then reveals the existence of topological edge states in the band gap, as well as a mobility edge (the border state that separates extended and localized states in the bulk of the spectrum) [27]. Finally, considering some practical requirements of any experimental realization, allows us to give a detailed picture of the electron dynamics throughout the process of adiabatic (Thouless) charge pumping. The comparison of the charge ordered system to the IQHE, allows us to clarify the nature of transport in both systems.

2. The model

We consider a tight-binding model for a finite charge ordered chain with open boundary conditions, containing $N$ atoms and $Nn$ spinless electrons. The filling factor $n$ is a common fraction, and the Hamiltonian is given by:

$$H = \sum_{j=1}^{N-1} \left[ -t \left( c_j^\dagger c_{j+1} + c_{j+1}^\dagger c_j \right) + Vc_j^\dagger c_j c_{j+1}^\dagger c_{j+1} \right].$$

Here, $t > 0$ is the hopping amplitude and $V > 0$ is the strength of the nearest-neighbor Coulomb interaction. The operator $c_j^\dagger$ ($c_j$) creates (annihilates) an electron at position $x = ja$, where $a$ is the lattice constant.

The interaction term in equation (1) is treated within mean-field theory using the Ansatz:

$$\langle c_{j+1}^\dagger c_{j+1} + c_{j-1}^\dagger c_{j-1} \rangle / 2 \simeq \langle c_j^\dagger c_j \rangle \propto \cos(2\pi nj + \phi).$$

Here, $\phi$ is the phase that determines the position of the CDW with respect to the lattice. After substituting the Ansatz in equation (1), the real-space mean-field Hamiltonian can be written as:

$$H = \begin{pmatrix} c_1^\dagger & c_2^\dagger & \ldots & c_N^\dagger \end{pmatrix} \times h \times \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_N \end{pmatrix}, \quad h = \begin{pmatrix} \epsilon_1 & -t & 0 & \ldots & 0 \\ -t & \epsilon_2 & -t & \ldots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \ldots & \epsilon_N \end{pmatrix},$$

with $\epsilon_j \propto \cos(2\pi nj + \phi)$.

Throughout the following, we use the parameter values $n = 1/3$, $V/t = 5$, and $N = 63$. Variations in the number of sites $N$ do not qualitatively affect the results. Note that with these parameters, CDW formation gives rise to three energy bands with 21 energy levels each, separated by two band gaps. The energy spectrum is obtained by numerically diagonalizing the Hamiltonian in equation (3), and is schematically shown in figure 1.

3. Edge states and Mobility edge

Among the eigenfunctions of the Hamiltonian matrix in equation (3), the bulk and edge states can be easily distinguished. The bulk wave functions can be understood as the eigenstates of a particle in a box, dressed with the periodic modulation of the charge-density waves. The edge states on the other hand, are exponentially localized on one of the end points of the chain.
Figure 1. Schematic energy spectrum of the CDW system with open boundary conditions. The magenta and blue lines represent edge states and mobility edges respectively, while dashed lines indicate how the edge state traverses the bulk bands before becoming the mobility edge. The Fermi energy is denoted $E_F$ on the vertical axis.

Notice that edge states appear in the lowest energy gap as the 21\textsuperscript{st} and 22\textsuperscript{nd} states, and in the higher energy gap as the 42\textsuperscript{nd} and 43\textsuperscript{rd} states.

In the ground state at one-third filling the highest occupied state is the 21\textsuperscript{st}. Inspection of figure 2(a) shows that upon varying $\phi$ this state changes from an edge state localized on one side of the chain to an edge state on the opposite side. Namely, for $0 \leq \phi \lesssim 1$, the electron is localized on the top side of the chain ($j = 63$). Then, for $1 \lesssim \phi \lesssim 3$, it propagates through the bulk and for $3 \lesssim \phi \lesssim 5$ it emerges on the bottom side ($j = 1$). For $5 \lesssim \phi \leq 2\pi$, it reappears again on the top side, without having propagated through the bulk. Similar behavior is seen for the 22\textsuperscript{nd} state.

Moreover, comparing the first two wave functions in the second energy band (the 22\textsuperscript{nd} and 23\textsuperscript{rd}) shows that they both change character as the edge state enters the bulk. For $\phi \lesssim 4$, the 23\textsuperscript{rd} state has a single node (mint color region around $j = 30$ in figure 2(b)), analogous to the first-excited state of a particle in a box. In contrast, for $\phi \gtrsim 4$ the charge distribution of the 23\textsuperscript{rd} state has no nodes, corresponding to the ground state of a particle in a box. The change in character can be understood by noticing that $\psi_{22}$, which was a propagating bulk state for $\phi \lesssim 4$, becomes an edge state at $\phi \gtrsim 4$. The next state in line can then take over the role of nodeless particle in a box ground state. This pattern in fact repeats throughout the bulk band, and all bulk states up to the middle of the band shift their character by one node as the edge state enters the bulk spectrum. This observation yields a natural connection between the localized and extended bulk states. That is, a single special, delocalized state can be recognized to exist among the bulk states in the second energy band, as shown in figure 2(c). This mobility edge sits precisely in the middle of the second band, and is connected to the edge states at other values of $\phi$ through the avoided crossings that we observe as a shift in the character of the bulk states.

A mobility edge is also found in the 11\textsuperscript{th} energy level, for $1 \lesssim \phi \lesssim 3$, and in the 53\textsuperscript{rd} state, for $4 \lesssim \phi \leq 2\pi$. In each case, it is the state precisely in the middle of a band. For an even number of sites $N$, there are two wave functions in the middle of each energy band, and both contain delocalized states.

The picture of edge states mixing with all bulk states, shifting them, and propagating through the bulk spectrum until they become a mobility edge in the center of the band, is further supported by the observation that the charge distributions of all bulk states contain remnants of the edge states after being traversed by them, as can be seen for example in figure 2(b) around $\phi \approx 4$. 

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Figure 2. The squared amplitude of the different wave function as a function of phase $\phi$ and position $j$ along the CDW chain. a) Edge state $|\psi_{21}|^2$, which is localised at the edges of the chain for $\phi \lesssim \pi/3$ and $\phi \gtrsim \pi$; b) Bulk state $|\psi_{23}|^2$; c) Mobility edge $|\psi_{32}|^2$, which is completely delocalised for $0 \lesssim \phi \lesssim \pi/3$ and $\pi \lesssim \phi \lesssim 4\pi/3$.

4. Adiabatic pumping

In any practical experimental implementation the topological transport across a CDW wire, the separated edges of the chain will typically be connected by a wire, so that the produced current can be measured. Such a connection may be added to the Hamiltonian of equation (3), by adding the terms $-\tilde{t}_c c_{0} \psi_{N-1}$ and $-\tilde{t}_c c_{N-1} \psi\psi_{0}$ in the matrix. Here, the hopping constant $\tilde{t}$ is taken to much be smaller than the in-chain hopping $t$. Adiabatic pumping, during which the full CDW system always stays in its instantaneous ground state, then involves an electron localized on one side of the chain traveling through the wire before arising on the opposite side (as indicated in figure 2 (a)). This can be seen directly in the spectrum by the fact that connecting the edges by a wire results in a gap $\propto \tilde{t}$ opening between the edge states in the band gap. This gap in fact is what allows the system to stay in the ground state, despite the adiabatic variation of $\phi$. Moreover, even if the evolution is not quite adiabatic, and the electron jumps across the energy gap between the edge states (e.g. from $\psi_{21}$ to $\psi_{22}$ at $\phi \simeq 5.3$), it may relax back to the edge state with lower energy $\psi_{21}$ by traversing the wire. The adiabatic charge transport is an incarnation of the topological Thouless pump. The number of transferred electrons per cycle of the pump equals the sum of Chern numbers for all occupied bands, as it does in the IQHE.

To clarify how the Chern number can be straightforwardly calculated for charge ordered materials, consider a one-third filled chain with periodic boundary conditions. The one-third filling implies the chemical potential lying within the lowest energy gap for all values of $\phi$. The periodic boundary conditions remove all edge states from the spectrum, and allows the Chern number to be calculated as an integral over the periodic BZ.

The Hamiltonian for one-third filling and closed boundary conditions can be written as

$$H = \sum_k h(k),$$

with:

$$h(k) = \begin{bmatrix}
-2t \cos ka & \tilde{c} e^{i\phi} & \tilde{c} e^{-i\phi} \\
\tilde{c} e^{-i\phi} & -2t \cos(ka + 2\pi/3) & \tilde{c} e^{i\phi} \\
\tilde{c} e^{i\phi} & \tilde{c} e^{-i\phi} & -2t \cos(ka + 4\pi/3)
\end{bmatrix}. \tag{4}$$

The amplitude of mean-field parameter $\tilde{c}$ may be assumed to be much smaller than $t$. This Hamiltonian has the same form as Harper’s equation, describing the IQHE, upon identifying $k \to k_x$ and $\phi \to k_y$. Its energy spectrum is presented in figure 3.

The Chern number $c_m$ may now be computed as an integral of Berry curvature $\Omega_{k\phi}^m$ over the first BZ, calculated for the one occupied band of energy eigenstates:

$$\Omega_{k\phi}^m = \langle \partial_{k} \psi_m | \partial_{\phi} \psi_m \rangle - \langle \partial_{\phi} \psi_m | \partial_{k} \psi_m \rangle,$$

$$c_m = \frac{1}{2\pi i} \int_0^{2\pi} d\phi \int_{BZ} \Omega_{k\phi}^m dk. \tag{5}$$
Figure 3. Energy spectrum of the CDW system with closed boundary conditions.

The resulting Chern number is the topological index which characterizes the CDW and yields the number of electrons in the $m^{th}$ band that are adiabatically transported around the chain upon varying the phase $\phi$ over one period.

Because the Chern number is a topological quantity, it is invariant under transformations the Hamiltonian which affect both its eigenvalues and the eigenvectors, as long as the transformations don’t cause any band inversions. We use this fact to calculate the Chern number for the CDW in a straightforward manner. All that is needed is to consider the three special points $k_1 = -\pi/3a$, $k_2 = 0$ and $k_3 = \pi/3a$, at which band inversions might occur. At these points, the eigenstates can be approximated by leaving all off-diagonal elements out of the Hamiltonian, except for those two that connect the two states which are nearly degenerate. Since one-third filling involves only the lowest band, we are interested only in the near degeneracies at $k_1$ and $k_3$. Near the point $k_1$ the lowest energy eigenstate can then be approximated by writing:

$$h(k_1, \phi) \approx \begin{bmatrix} -t & \tilde{c}e^{i\phi} & 0 \\ \tilde{c}e^{-i\phi} & -t & 0 \\ 0 & 0 & t \end{bmatrix}, \quad |\psi_1\rangle \equiv |\psi(k_1, \phi)\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -e^{-i\phi} \\ 0 \end{pmatrix}. \quad (6)$$

For point $k_3$, we should instead consider:

$$h(k_3, \phi) \approx \begin{bmatrix} -t & 0 & \tilde{c}e^{-i\phi} \\ 0 & 2t & 0 \\ \tilde{c}e^{i\phi} & 0 & -t \end{bmatrix}, \quad |\psi_2\rangle \equiv |\psi(k_3, \phi)\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ -e^{i\phi} \end{pmatrix}. \quad (7)$$

In between these two near degeneracies, at $k = 0$, the lowest energy state is far from all other states, and may be approximated as $|\psi(k_2, \phi)\rangle = (1, 0, 0)^T$.

The eigenvectors in equations (6) and (7) are determined up to an arbitrary phase factor only. The calculation of the Chern number will become particularly straightforward if we divide the BZ into two parts, $S_1 \in [k_1, k_2]$ and $S_2 \in [k_2, k_3]$, and choose different conventions for the phase of the eigenvectors in each region. The lowest energy eigenstates can then be defined to be:

$$|\Psi_1(k, \phi)\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} \sqrt{2 - \alpha^2(k)} \\ \alpha(k) e^{-i\phi} \\ 0 \end{pmatrix}, \quad |\Psi_2(k, \phi)\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} \sqrt{2 - \beta^2(k)} \\ 0 \\ -\beta(k) e^{i\phi} \end{pmatrix}. \quad (8)$$

Here, $\alpha(k)$ is some real function with values 1 and 0 at momenta $k_1$ and $k_2$ respectively, and $\beta(k)$ is a real function with values 0 and 1 at momenta $k_2$ and $k_3$ respectively. The formula for the Berry curvature given in (5) then yields:

$$S_1 : \Omega_{k\phi}^1 = -i\alpha' \alpha, \quad S_2 : \Omega_{k\phi}^1 = i\beta \beta'. \quad (9)$$
The Chern number can be found to be:

\[ c_1 = \frac{1}{2\pi i} \int_0^{2\pi} d\phi \left[ -i \int_{k_1}^{k_2} \alpha' \alpha dk + i \int_{k_2}^{k_3} \beta' \beta dk \right] = +1. \]  

(10)

This result shows that the CDW acts as a Thouless pump, by transferring one electron through the wire connecting its ends as the charge order slides by one wavelength. This is the CDW-analogue of the well-known result for the IQHE [15].

5. Conclusion

In this work, we consider topological charge transport, or Thouless pumping, in charge ordered materials. These systems can be mapped directly onto the well-known topological transport in an IQHE cylinder, but they have the advantage that there is no electromagnetic gauge freedom. This allows for a direct visualization of the electron dynamics during an adiabatic pumping cycle. It also allows for a straightforward identification of the mobility edge in the bulk spectrum, and reveals its connection to the topological edge states. Finally, in the charge ordered systems, the Chern number characterizing the adiabatic pump at any given filling fraction can be found by direct integration of the Berry curvature.

The real-space structure of CDWs can be directly imaged in experiments. For example, using the scanning tunneling microscope (STM) to determine the topography of a surface, one observes the modulations in atomic structure and charge-density imposed by the CDW [28, 29, 30, 31, 32]. This gives direct access to both the amplitude and phase of the CDW order parameter. Photonic wave guides offer an alternative route, and have recently been used to show topological transport across a quasicrystalline chain [33], which can be mapped onto an incommensurate version of the sliding CDW [12]. We hope that our results will motivate further experimental research in this field.

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References

[1] von Klitzing K, Dorda G and Pepper M 1980 Phys. Rev. Lett. 45 494
[2] Bernevig B A, Hughes T L and Zhang S-C 2006 Science 314 1757
[3] Koenig M, Wiedmann S, Bruene C, Roth A, Buhmann H, Molenkamp L W, Qi X-L and Zhang S-C 2007 Science 318 766
[4] Kane C L and Mele E J 2005 Phys. Rev. Lett. 95 226801
[5] Qi X-L and Zhang S-C 2010 Phys. Today 63 33
[6] Hasan M Z and Kane C L 2010 Rev. Mod. Phys. 82 3045
[7] Qi X-L and Zhang S-C 2011 Rev. Mod. Phys. 83 1057
[8] Thouless D J, Kohmoto M, Nightingale M P and den Nijs M 1982 Phys. Rev. Lett. 49 405
[9] Harper P G 1955 Proc. Phys. Soc. Lond. A 68 874
[10] Holstätter P D 1976 Phys. Rev. B 14 2239
[11] Peierls R 1930 Ann. d. Phys. Leipzig 4 121
[12] Flicker F and van Wezel J 2015 EPL (Europhysics Letters) 111 37008
[13] Ozawa T, Price H M and Carusotto I 2015 Phys. Rev. A 92 023609
[14] Halperin B I 1982 Phys. Rev. B 25 2185
[15] Hatsugai Y 1993 Phys. Rev. Lett. 71 3697
[16] Laughlin R B 1981 Phys. Rev. B 23 5632
[17] Thouless D J 1983 Phys. Rev. B 27 6083
[18] Altshuler B L and Glazman L I 1999 Science 283 1864
[19] Switkes M, Marcus C M, Campman K and Gossard A C 1999 Science 283 1905
[20] Moskalets M and Buttiker M 2002 Phys. Rev. B 66 205320
[21] Maruyama I and Hatsugai Y 2009 J. Phys.: Conf. Ser. 150 022055
[22] Nakajima S, Tomita T, Taie S, Ichinose T, Ozawa H, Wang L, Troyer M and Takahashi Y 2016 Nat. Phys. 12 296
[23] Lohse M, Schweizer C, Zilberberg O, Aidelsburger M and Bloch I 2016 Nat. Phys. 12 350
[24] Ma W, Zhou L, Zhang Q, Li M, Cheng Ch, Geng J, Rong X, Shi F, Gong J and Du J 2018 Phys. Rev. Lett. 120 120501
[25] Dolgopolov V T, Shashkin A A, Zhitenev S I, Dorozhkin N B and von Klitzing K 1992 Phys. Rev. B 46 12560
[26] Vorob’ev A B, Prinz V Ya, Yukecheva Yu S, Toropov A I 2004 Physica E 23 171
[27] Basko D M, Aleiner I L and Altshuler B L 2006 Ann. Phys 321 1126
[28] Snijders P C, Rogge S and Weiting H H 2006 Phys. Rev. Lett. 96 076801
[29] Brun C, Wang Zh-Zh, Monceau P and Brazovskii S 2010 Phys. Rev. Lett. 104 256403
[30] Xi X, Zhao L, Wang Z, Berger H, Forro L, Shan J and Mak K F 2015 Nat. Nano. 10 765
[31] Novello A M, Hildebrand B, Scarfato A, Didiot C, Monney G, Ubaldini A, Berger H, Bowler D R, Aebi P and Renner Ch 2015 Phys. Rev. B 92 081101
[32] Ugeda M M et al. 2016 Nat. Phys. 12 92
[33] Kraus Y E, Lahini Y, Ringel Z, Verbin M and Zilberberg O 2012 Phys. Rev. Lett. 109 106402