Two-dimensional sliding charge density waves and their protected edge modes

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We propose and study a two-dimensional (2D) charge density waves (CDW) phase, which is constructed from an array of weakly coupled one-dimensional (1D) sliding CDW wires whose phases shift from one wire to the next. We show that the fully gapped bulk CDW has topological properties, characterized by a nonzero Chern number, that imply protected edge modes within the bulk gap. The edge modes exhibit spectral pseudo-flow as a function of position along the edge, and are thus dual to chiral edge modes of Chern insulators with their spectral flow in momentum space. Furthermore, we show that these sliding CDW edge modes are stable against small inter-wire coupling. Our predictions can be tested experimentally in quasi-1D CDW compounds such as Ta3Se8I.

An insightful way to think about quantum Hall phases is in terms of an array of weakly coupled 1D sliding Luttinger liquids (SLL) [1–3]. Each SLL consists of gapless excitations around its Fermi points $k_0 \pm k_F$, where the origin in momentum space $k_0$ is a priori a gauge choice. When coupling identical wires that are displaced in the $x$-direction and extend along the $y$-direction, the difference $\delta k$ between their respective $k_0$ is an observable proportional to the flux density (i.e., the perpendicular magnetic field) between them (see Fig. 1a). A wire array built in this way is then akin to a sequence of Luttinger liquids with dispersions displaced by $k_0(x) = x\delta k$. Weak coupling between the wires opens a spectral gap in the bulk and the system enters a quantum Hall phase with chiral edge modes and quantized Hall conductivity (see Fig. 1b,c).

In this work, we contrast this construction of a topological phase from a SLL with a construction of a 2D phase of sliding charge density waves (CDW) [4]. The CDW modulation in a 1D wire can be characterized by a potential such as $\cos(Q_y y + \phi_0)$, where $Q_y$ is the CDW wavevector and $\phi_0$ is a phase that, in the case of breaking a continuous translation symmetry, is associated with the Goldstone mode of the sliding CDW. In contrast to $k_0$ in the SLL, $\phi_0$ is not a gauge freedom of the 1D system, but determines the real-space origin of the charge density pattern. Our objective is to study the properties of an array of weakly coupled sliding CDWs whose phases are shifted as $\phi_0(x) = Q_x x$ (see Fig. 1d). We find a duality between the edge modes of the SLL and the sliding CDW: In a ribbon geometry, the former has edge modes with spectral flow as a function of position along the edge, while the latter has edge modes with spectral pseudo-flow [8] as a function of position along the edge (see Fig. 1e,f).

In addition, we find that the sliding CDW edge modes are substantially robust against inter-wire coupling.

Fig. 1. Duality between the coupled sliding Luttinger liquids (left) and coupled sliding CDWs (right). (a) Schematic of a planar array of weakly coupled 1D SLLs under a uniform flux density. It leads to a Chern insulator. The dashed lines separate areas with unit magnetic flux $\Phi_0$. (b) Chiral edge modes (red) of the Chern insulator within the bulk insulating gap (black). They exhibit spectral flow as a function of momentum along the edge. (c) Chiral edge modes in the bulk gap in position space, which are translation-invariant along the edge. (d) Schematic of the 2D sliding CDW, which is constructed from an array of weakly coupled 1D CDW wires along the $y$-direction whose phases shift with $x$-position, as depicted by the changing color in the background. (e) Sliding CDW edge modes with energies within the CDW gap. The edge modes are dispersion-free in momentum $k_x$ along the edge. (f) Sliding CDW edge modes in position space. They exhibit spectral pseudo-flow as a function of position along the edge.
Our study is not purely theoretically motivated, but aims to model the key aspects of the CDW compound Ta$_2$Se$_3$I. In line with the sliding CDW picture, Ta$_2$Se$_3$I consists of weakly coupled chains. It is known to undergo a CDW transition at $T_{\text{CDW}} \approx 260$ K [9–16], developing a sizable gap that experiments determined to be between 100 and 500 meV, with a small ordering wave vector that amounts to $Q_y \approx 0.095\pi/c$ and $Q_z \approx 0.054\pi/a$, where $c$ and $a$ are the lattice constants [15, 17]. Recent studies highlighted a multitude of Weyl nodes that are induced through spin-orbit coupling in the low-energy electronic structure of Ta$_2$Se$_3$I above $T_{\text{CDW}}$ and their implications for possible axion physics in the CDW phase [14, 15]. However, experimental evidence for a three-dimensional topological (axionic) nature of the CDW state is lacking [17]. Here, we advocate a much simpler model of a sliding CDW phase for Ta$_2$Se$_3$I, for which spin-orbit coupling is unimportant. Our theory makes the experimentally testable prediction of boundary states at certain surfaces or step edges of this material.

We start by defining a two-orbital model on a 2D rectangular lattice in the presence of a CDW modulation, $\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_{\text{CDW}}$ with

$$\mathcal{H}_0 = \frac{1}{2} \sum_{\mathbf{r}} \left( t_y \Psi^\dagger_{\mathbf{r}+\hat{y}} \sigma_y \Psi_{\mathbf{r}} + t_x \Psi^\dagger_{\mathbf{r}+\hat{x}} \sigma_x \Psi_{\mathbf{r}} + \text{h.c.} \right),$$

where $\Psi^\dagger_{\mathbf{r}} = (c^\dagger_{1\mathbf{r}}, c^\dagger_{2\mathbf{r}})$ with $c^\dagger_{\sigma \mathbf{r}}$ creating an electron with orbital $\sigma \in \{1, 2\}$ at position $\mathbf{r} = (x, y)$. $\hat{x}$ and $\hat{y}$ are the nearest-neighbor vectors in the $x$- and $y$-directions, respectively, and h.c. represents the Hermitian conjugate counterpart. $\sigma_x, \sigma_y$, and $\sigma_z$ are Pauli matrices acting on the two orbitals. We consider the situation where the two orbitals are of $s$ and $d_{xy}$ types, respectively. Thus, the two orbitals do not couple via on-site or nearest-neighbor hopping terms if $x \rightarrow -x$ and $y \rightarrow -y$ mirror symmetries above the CDW transition are imposed. Furthermore, the orbital character suggests hopping amplitudes with opposite signs, thus motivating the form of Hamiltonian (1). Note that the model can be viewed as an array of 1D parallel wires that are displaced in the $x$-direction and extend along the $y$-direction. Thus, $t_y$ and $t_x$ correspond to the hopping strength along the wires and the inter-wire coupling strength, respectively (see Fig. 1d). The lattice constants are taken to be unity. In the normal state (without CDW), the model is gapless with band crossings protected by the symmetries. In this work, we focus on the parameter regime $0 \leq t_x < t_y$, such that the model approximates the relevant electronic structure of Ta$_2$Se$_3$I. The energy bands of $\mathcal{H}_0$ are given by $\varepsilon_{\pm}(\mathbf{k}) = \pm [t_y \cos(k_y) + t_x \cos(k_x)]$, where $\mathbf{k} = (k_x, k_y)$ is the 2D momentum. The bands cross around $k_y = \pm \pi/2$ along the $k_y$-axis and the Fermi surfaces take ribbon shapes in the $k_x$-$k_y$ plane (see Fig. 2), in agreement with those observed in Ta$_2$Se$_3$I [13, 16, 18].

The CDW modulation can be described as a spatially periodic local potential,

$$\mathcal{H}_{\text{CDW}} = V \sum_{\mathbf{r}} \cos(Q_y y + Q_x x + \phi) \Psi^\dagger_{\mathbf{r}} M \Psi_{\mathbf{r}},$$

where $V$ is the strength, and the CDW wavevector $Q_y$ along each wire as well as the phase shift $Q_x$ in neighboring wires are related to the wavelengths $\lambda_{x/y}$ as $Q_{x/y} = 2\pi/\lambda_{x/y}$. We are assuming a limit where the CDW wavelengths are large integers compared to the lattice constants $\lambda_{x/y} \gg 1$ [19]; $\phi$ is the global constant phase of the CDW. We focus on inter-orbital CDW modulations characterized by a matrix $M \in \{\sigma_x, \sigma_y\}$ which open bulk gaps in the low-energy regime, as we will discuss in detail below [20]. For illustration, we take $M = \sigma_x$, $\lambda_y = 21$, $t_y = 1.5$ eV and $V = 0.3$ eV unless specified otherwise.

To elucidate the essential physics, we first consider the limit of decoupled wires ($t_x = 0$) which allows us to calculate each 1D wire separately. Note that in this limit, all wires are identical except for their $y$-dependent CDW phases $\phi_0(x) = Q_x x + \phi$. To explore the topological properties of the system, we impose periodic boundary conditions in the $y$-direction. Due to the super-periodic CDW potential with a large period $\lambda_y$, the spectrum is split into $2\lambda_y$ bands in the reduced Brillouin zone, as shown in Fig. 3a. Clearly, two bulk gaps of size $V$ appear at $\varepsilon_{\pm} \approx \pm t_y \sin(\pi/\lambda_y)$, respectively, which separate three parts of the spectrum: four bands in the middle, $\lambda_y - 2$ bands at the top and the other $\lambda_y - 2$ bands at the bottom. The bulk bands disperse in $k_y$, whereas they are flat in $\phi$ (see Fig. 3b). Note that the spectrum is periodic in both $k_y$ and $\phi$. A topological characterization of the system can be obtained in terms of the Berry phase in the compact $k_y$ and $\phi$ space [21]. Specifically, for each spectral gap, the Chern number can be computed as [22]

$$\nu = \int_{-\pi/\lambda_y}^{\pi/\lambda_y} dk_y \int_{-\pi}^{\pi} d\phi \text{Tr}[\partial_{k_y} \mathbf{A}_\phi - \partial_\phi \mathbf{A}_{k_y}],$$

where $\mathbf{A}_j$ with $j \in \{k_y, \phi\}$ is the non-Abelian Berry connection $\mathbf{A}_j = i \Psi^\dagger \partial_j \Psi$ which is a square matrix and based on the multiplet of eigenstates with energy below the gap.
The nontrivial Chern numbers indicate the appearance of mid-gap edge modes when open boundaries are imposed in the $y$-direction, at least for a certain range of $\phi$ of the wire. To show this explicitly, we consider $L_y = 85$ lattice sites with open boundary conditions, the Fermi energy $E_F = -t_y \sin(\pi/\lambda_y)$, and calculate the local density of states (LDOS) as a function of position $y$ along the wire (see Fig. 3c). Clearly, away from the boundary, the LDOS shows a bulk gap around $E_F$ that varies periodically with position, which is consistent with the scanning tunnelling microscopy experiments on Ta$_2$Se$_8$I [16–18]. The period in the LDOS is $\lambda_y/2$, half of that in the CDW potential. Inside the gap, exponentially localized edge modes appear for a large range of $\phi$. The energies of the edge modes at opposite boundaries are generally different. They depend sensitively on $\phi$, in contrast to the bulk gaps that are constant in $\phi$. Crucially, in the 2D array, the phases $\phi_0(x)$ of the wires shift in the $x$-direction. The $\phi_0$ dependence of the edge modes indicates the spectral pseudo-flow as a function of position along the edge, which is confirmed numerically in Fig. 4d. The Chern number $\nu$ determines the number of pseudo-flow modes within a wavelength $\lambda_x$ along the edge [23].

In the limit where the wires are decoupled in the $x$-direction ($t_x = 0$), both the bulk and edge spectra are flat in the reduced $k_x$ space (see Fig. 4a). This indicates that the edge modes are immobile in the $x$-direction, in stark contrast to the chiral edge modes in the Chern insulator that carry current. Moreover, due to the shifted phases in the CDW wires, at each boundary, up to $\lambda_x$ edge bands appear in the $k_x$ space. The edge modes with different energies are located at different lattice sites within a wavelength $\lambda_x$ along the edge, which again indicates the unique edge spectral pseudo-flow in the 2D sliding CDW system.

Next, we consider finite inter-wire coupling $t_x$ and show that the main features of the sliding CDW discussed above are remarkably stable in the presence of the inter-wire coupling. For illustration, in Figs. 4a–c, we consider $\lambda_x = \lambda_y = 21$ and $L_y = 421$, and calculate the energy spectrum for increasing $t_x$, with periodic and open boundary conditions in the $x$- and $y$-directions, respectively. We find that as $t_x$ increases, the CDW gap is reduced and close completely after a critical strength $t_x = t_c$. Figure 4f plots the size of the CDW gap $\Delta_{CDW}$ as a function of $t_x$. Clearly, $\Delta_{CDW}$ decreases almost linearly with increasing $t_x$ (see the thick lines in Fig. 4f). Moreover, for a larger CDW wavelength $\lambda_x$, the reduction of $\Delta_{CDW}$ by $t_x$ is slower and hence a larger $t_c$ is observed (see Fig. 4g). The critical strength $t_c$ also increases with increasing $V$. Notably, for $\lambda_x > 5$, $t_c$ is comparable and even larger than $V$, i.e., $t_c \gtrsim V$. As a consequence of the reduction of $\Delta_{CDW}$, some edge bands are merged with the bulk continuum. Thus, edge modes can be observed at fewer sites along the edge (see Fig. 4b,e). However, the remaining edge modes with energy closer to the Fermi energy $E_F$ are only slightly extended in the $y$-direction. Therefore, for large $\lambda_x$ and $V$, the system with sizable CDW gaps and sliding edge modes can persist up to considerable inter-wire coupling.

While the CDW gap $\Delta_{CDW}$ are obviously reduced by the inter-wire coupling, the energies of the edge modes remain almost dispersion-free in $k_x$ even for considerable $t_x/t_y$ as long as the edge modes persist in the bulk gap. In Fig. 4f, we also compute one of the edge bandwidths $\delta E_{edge}$ as a function of $t_x$. We clearly see that $\delta E_{edge}$ grows as a power-law function of $t_x$. However, it is always several orders of magnitude smaller than $\Delta_{CDW}$ (whose magnitude is of the same order of $V$). Overall, the flatness of the edge bands against $k_x$ tends to be more pronounced for an odd and larger value of $\lambda_x$. These features can be attributed to the existence of the spectral pseudo-flow of the edge modes and that, for odd (even)
Fig. 4. (a–c) Energy spectra for inter-wire coupling strengths $t_x = 0, 0.3t_y$, and $0.8t_y$, respectively. The bulk continuum and the discrete edge bands are indicated by gray and red color, respectively. Periodic and open boundary conditions are imposed in both the $x$- and $y$-directions, respectively. (d) and (e) LDOS at low energies for $t_x = 0$ and $0.3t_y$, respectively. (f) Size of the CDW gap $\Delta_{CDW}$ (thick lines) and one of the edge bandwidths $\delta E_{edge}$ (circle lines) as functions of $t_x$, respectively. $\Delta_{CDW}$ decreases monotonically with increasing $t_x$ and closes after a critical strength $t_x = t_c$. $\delta E_{edge}$ grows in a power-law manner as $t_x$ increases, but is always orders of magnitude smaller than $\Delta_{CDW}$. We choose three different wavelengths $\lambda_x = 10$ (blue), 15 (orange) and 21 (green) for illustration. (g) $t_x$ as a function of $\lambda_y$ for $V = 0.2$ eV, 0.3 eV and 0.5 eV, respectively, $t_x$ increases as $\lambda_y$ or $V$ increases. $L_y = 421$ and $\phi = 0$ in all panels, $\lambda_x = 21$ and $L_x = 10\lambda_x$ in (d,e), and other parameters are the same as those in Fig. 3.

$\lambda_x$, edge modes at the same energy level are spatially separated by a distance $\lambda_y (\lambda_x/2)$. The flatness of the edge bands further indicates that the edge modes are immobile even in the presence of the hopping (i.e., inter-wire coupling $t_y$) in the edge direction.

Although in the above discussion we illustrated only the case with the inter-wire coupling diagonal in orbital space (i.e., characterized by $T = \sigma_2$), we stress that the effects are qualitatively the same for other forms of inter-wire coupling (e.g., characterized by a general $2 \times 2$ Hermitian matrix) [24]. We have also verified that small deviations of the band crossing points (in the absence of CDW) from $k_y = \pm \pi/2$ and a difference between the hopping amplitudes of the two orbitals do not alter our main results qualitatively [24]. Finally, it is worth noting that the sliding CDW with finite inter-wire coupling can be characterized by the same topological number as in the decoupled limit, since the two are adiabatically connected without a gap closure.

We now briefly discuss the experimental relevance of our predictions in the candidate material Ta$_2$Se$_4$I which consists of 1D TaSe$_4$ chains weakly coupled by van der Waals interaction. Recently, on the (110) surface of Ta$_2$Se$_4$I, large surface gaps with clear in-plane CDW modulations have been observed [16–18]. The CDW patterns have large CDW wavelengths ($\lambda_x/y \sim 17–25$ nm) both along and perpendicular to the chains. The CDW gaps ($\Delta_{CDW} \sim 0.1–0.5$ eV) are smaller than the energy scale of intra-chain hopping ($t_y \sim 1$ eV), but stronger than the van der Waals interaction ($t_x \sim 0.05$ eV) [13, 15–17]. These observations agree with the parameter regime of our 2D sliding CDW. Thus, along the boundaries or step edges that are perpendicular to the TaSe$_4$ chains, we predict the existence of edge modes with spectral pseudo-flow. Such crystal terminations could be prepared with focused ion beam manipulation [25, 26]. Note that compared to the theories involving Weyl physics [14, 15], our theory does not require spin-orbit coupling and is focused on a larger energy scale. We also expect our theory to be implementable in other quasi-1D CDW materials [27–32] such as TaTe$_4$ where desired CDW patterns on specific surfaces have been reported [33, 34].

To summarize, we have proposed a 2D sliding CDW phase with topologically protected edge modes inside the bulk gaps. In a ribbon geometry, the edge modes are immobile and exhibit spectral pseudo-flow as a function of position along the edge, constituting a duality compared to the chiral edge modes of Chern insulators (i.e., the SLL) which show spectral flow as a function of momentum. We have shown that the edge modes are substantially robust against inter-wire coupling. Our theory can be applied to quasi-1D CDW compounds such as Ta$_2$Se$_4$I.

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Supplemental material for "Two-dimensional sliding charge density waves and their protected edge modes"

In this Supplemental Material, we analyze the inverse participation ratio of edge modes (Sec. I), the results for other forms of inter-wire coupling (Sec. II), under small deformations of the normal electronic structure (Sec. III), and the case with Chern number $\nu = \pm 1$ (Sec. IV).

Appendix I: Inverse participation ratio of edge modes

To better show the localization properties of the edge modes in the presence of inter-wire coupling, in Fig. S1, we calculate the inverse participation ratio (IPR) of one edge mode with energy close to $E_F$. The inter-wire coupling slightly spreads the edge mode to two neighboring sites along the edge direction, thus reducing the IPR. However, when the edge mode persists in the bulk gap, it is clear to see that the edge mode has considerable IPR. This result indicates its strong localization at the edge. For large $\lambda_x$, the IPR only vanishes abruptly when the edge mode is merging into the bulk. Similar features appear for other edge modes and they are independent of the global phase $\phi$.

![Fig. S1. IPR of one of the edge modes as a function of inter-wire coupling strength $t_x$ for $\lambda_x = 10, 21$ and 32, respectively.](image)

Appendix II: Results for other forms of inter-wire coupling

In the main text, we discussed the case with the inter-wire coupling characterized by matrix $T = \sigma_z$, which is most relevant to the candidate material Ta$_2$Se$_8$I. In this section, we show that the main results are more general and hold for any form of inter-wire coupling (described by a general $2 \times 2$ Hermitian matrix). Note that a general inter-wire coupling may mix the two orbitals. However, for small coupling strength $t_x$, the model in the normal state remains in a metallic phase with band crossing points. A general $2 \times 2$ Hermitian matrix can be written as a linear combination of $\sigma_0$, $\sigma_x$, $\sigma_y$ and $\sigma_z$. To address the problem comprehensively, we present the results for the complementary cases with $T = \sigma_0$, $\sigma_x$ and $\sigma_y$, respectively (see Figs. S2 and S3). Similar to the main text, we choose the experimentally relevant parameters, namely, $t_y = 1.5$ eV, $V = 0.3$ eV and $\lambda_x = \lambda_y = 21$. We clearly see that in all the cases, the CDW gap is reduced by increasing inter-wire coupling strength $t_x$ and vanish after a large critical strength $t_x = t_c$. This means that the sizable CDW gap persists up to strong $t_x = t_c$ (i.e., with the magnitude in the same order as the CDW
Fig. S3. Size of the CDW gap $\Delta_{CDW}$ as a function of $t_x$ for $T = \sigma_0$, $\sigma_x$ and $\sigma_y$, respectively. The size $\Delta_{CDW}$ decreases monotonically with increasing $t_x$ and vanishes after a large critical $t_x = t_c$. Other parameters are the same as those in Fig. S2.

Appendix III: Results under small deformations of the normal band structure

In this section, we present the results for the cases where the band crossing deviated from $k_y = \pm \pi/2$ and the two orbitals have different hopping amplitudes (see Fig. S4a,d for the band structures), respectively. As illustrated in Fig. S4c,f, we see that the CDW gap $\Delta_{CDW}$ remains roughly the same for a wide range of the deviation of the crossing point $k_0$ and difference of the hopping amplitudes $\zeta$. Inside the CDW gap, multiple edge bands appear which are localized at different sites along the edge.

Appendix IV: 2D sliding CDW phase with Chern number $\nu = \pm 1$

In this section, we show that the 2D sliding CDW phase with the same main features but different Chern numbers $\nu = \pm 1$ is also possible. As a concrete example, we consider the following model

$$\mathcal{H}_0' = \frac{1}{2} \sum_r \left[ t_y (\Psi_r \sigma_x \Psi_r + \Psi_{r+y} (\sigma_x + i \sigma_y) \Psi_r + h.c.) + (t_x \Psi_{r+x} \Psi_{r} + h.c.) \right], \quad (IV1)$$

and the CDW potential

$$\mathcal{H}_{CDW} = V \sum_r \cos(Q_y y + Q_x x + \phi) \Psi_r \sigma_z \Psi_r. \quad (IV2)$$

As shown in Fig. S5, in the absence of CDW ($V = 0$), the model is gapless with band crossings at the band center $E = 0$. The CDW potential opens two CDW gaps of magnitude $V$ close to the band center. By employing the formula Eq. (3) in the main text, we find that the two gaps are characterized by $\nu = +1$ and $-1$, respectively. When imposing open boundary conditions in $y$ direction, the system has edge bands within the bulk gaps, which are flat in momentum $k_x$ along the edge. The edge bands with different energies are located at different sites along the edge, thus exhibiting a spectral pseudo-flow.

As determined by the Chern number, there is only one pseudo-flow mode within a wavelength $\lambda_x$ along the edge.
In Fig. S6, we consider the inter-wire coupling of different types and plot the size of the CDW gaps $\Delta_{\text{CDW}}$ as a function of the coupling strength $t_x$. We see that the influences of the inter-wire coupling are similar to that we discussed in the main text: the inter-wire coupling reduces $\Delta_{\text{CDW}}$ and closes the gap after a large critical strength. Thus, the 2D sliding CDW phase is stable to a considerable strength of inter-wire coupling.