Robust one-dimensionality at twin-grain-boundaries in MoSe₂

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We show that 1D electron states confined at twin-grain-boundaries in MoSe₂ can be modeled by a three-orbital tight binding model including a minimum set of phenomenological hopping terms. The confined states are robust to the details of the defect hopping model, which agrees with their experimental ubiquity. Despite a valley Chern number which is finite and opposite on both sides of the defect, there is no topological protection of the confined states. This turns out to be an essential feature to have only one confined electronic band, in agreement with experiments, instead of two, as the bulk-edge correspondence would imply. Modeling the confined state as a 1D interacting electronic system allows us to unveil a mobile quantum impurity type behavior at energy scales beyond the Tomonaga-Luttinger liquid with an interaction range which extends up to the lattice spacing, in excellent agreement with ARPES measurements.

Introduction.—One dimensional (1D) electronic systems are the host of many interesting phenomena, including the possible condensed matter realization of Majorana zero modes due to the non-trivial topology of the electron states [1], the observation, due to electron correlations [2], of both low-energy Tomonaga-Luttinger liquid (TTL) physics and higher-energy mobile quantum impurity model (MQIM) behavior, beyond TTL [3], as well as the observation of spin and charge separation at all energy scales [4], to mention a few. In a three-dimensional world, one-dimensionality is obviously not the rule. Fortunately, a variety of examples can be found in nature (or synthesized) — carbon nanotubes are a paradigmatic example [5], but also semiconducting nanowires, as for example InSb and InAs [1, 6], and assembled atom chains on surfaces [2, 7], have been on the spotlight recently, with prominent technological potential in some cases.

The advent of two-dimensional materials [8], in particular the realization of a new class known as semiconducting transition metal dichalcogenides (TMDs) [9], formula MX₂, where M is a transition metal (ex. Mo, W) and X is a chalcogen (ex. S, Se) [10, 11], allowed for a new type of 1D electron system: a confined state at the twin-grain-boundary (TGB) defect shown in Fig. 1(a). The presence of such 1D states inside the bulk gap, in excess of 1 eV, has been clearly demonstrated experimentally [12–15]. Their metallicity also became apparent, as well as intrinsic 1D behavior such as a Peierls transition originating a charge density wave order below T ≲ 250 K, as well as spin and charge separation characteristic of a correlated 1D system [4, 14].

In this paper, we show that the three-orbital tight binding (TB) model of Ref. [16], widely used to describe physics around the gap edges in TMDs, can be used to describe the confined 1D states at TGBs. A minimum set of phenomenological hoppings are included to couple the two sides of the TGB. The induced in-gap states are robust to the details of the defect hopping model, being present in its simplest version where only nearest-neighbor (NN) hoppings between d_{xy} orbitals are allowed. The respective spectrum is showed in Fig. 1(b), where a band of states localized at the TGB is clearly seen crossing the gap. The localized nature of the states is depicted in Fig. 1(c), where we show the probability density for a K-valley state. The valley Chern number, which changes

![Figure 1](attachment:image.png)

Figure 1: (a) MX₂ lattice with a TGB defect along the x direction. (b) Spectrum for a ribbon of MX₂ with a TGB in the middle, obtained with a single hopping parameter to couple the two sides of the TGB (see text). A band of electron states confined at the TGB is shown as a thick (orange) line. Thin (black) lines are bulk states and short-dashed (blue and orange) are other 1D states. (c) Probability density for an electron confined at the TGB in the K-valley direction.
sign across the boundary and takes values $C_e = \pm 1$, does not warrant topological protection of the 1D states. This is crucial to stabilize a single band at the TGB, in agreement with experiments and \textit{ab initio} simulations [14, 17, 18], as opposed to what would be implied by the Chern number change $|\Delta C_e| = 2$ [19]. The stability of the single band is, however, reminiscent of the Berry phase difference between the two sides of the TGB Zhu et al. [20]. Including interactions in the effective 1D system, and explicitly accounting for the effects of the finite range of the interaction between the MQIM charge degrees of freedom, improves the agreement with ARPES experiments beyond that reached in Ref. [4].

\textit{Tight-binding analysis}.—We model electrons in MoSe$_2$ using a M atom 3-orbital NN-TB Hamiltonian given by

$$H_0 = \sum_{i,\alpha} \sum_{\gamma,\gamma',\sigma} c^\dagger_{i,\gamma,\sigma} E^\sigma_{\gamma,\gamma'}(R_\alpha) c_{i+R_\alpha,\gamma',\sigma},$$

where $c^\dagger_{i,\gamma,\sigma}$ is an electron creation operator on lattice site $i$, M atom orbital $\gamma = d_x, d_{xy}, d_{x^2-y^2}$, spin $\sigma = \uparrow, \downarrow$, and $R_\alpha$ with $\alpha = 1, \ldots, 6$ are the six vectors connecting NN atoms as shown in Fig. 1(a). $E^\sigma_{\gamma,\gamma'}(R_\alpha)$ are hopping integrals as given in Ref. [42]. We write the TB Hamiltonian, including the TGB, as $H = H_R + H_R + H_{TGB}$, with $H_R \equiv H_0$ to the left of the TGB ($y < 0$) and $H_R \equiv \sigma_0 H_0 \sigma_0$, to the right ($y > 0$), where $\sigma_0$ is the reflection operator associated to the mirror transformation $y \rightarrow -y$ [see Fig. 1(a)], and $H_{TGB}$ couples left and right regions. $H_R$ can be written as in Eq. (1) with the NN hoppings reversed [see Fig. 1(a)]. $H_{TGB}$ is modeled in two ways: a simplified model, where only the NN hopping between M-atom $d_{xz}$ orbitals is allowed; and a more elaborated model, where three NN hopping terms are allowed across the TGB.

The results for the simplified model are shown in Fig. 2(a-c), respectively for hopping values $|\tilde{t}_{xz}| = 0.2, 0.6, 1.0$ eV, where we considered a ribbon with translational invariance along $x$-direction and $N_y = 100$ unit cells in the $y$-direction, transverse to the TGB. Panel 2(c) is the same as the one in Fig. 1(c). In the latter, the dashed blue line corresponds to edge states localized at the outer edges of the ribbon, so-called M-edges. These edge states, present in all panels of Fig. 2, have been studied elsewhere [16, 21, 22] and will be ignored here. In the limit $\tilde{t}_{xz} = 0$, the TGB is composed of two uncoupled X-edges, which also support edge states [23, 24]. In Fig. 2(a) it is seen that a finite $\tilde{t}_{xz}$ lifts the degeneracy of the two X-edge states. On increasing $\tilde{t}_{xz}$ [Figs. 2(b) and 2(c)], bonding and anti-bonding states are formed. The bonding state is pushed down in energy, particularly when the localization length is smaller ($k_x a \approx \pi$), and will be partially occupied.

The orbitals $d_{xz}$ and $d_{x^2-y^2}$ are the most important for the defect state. A more realistic model for $H_{TGB}$ considers three hoppings across the defect: direct hoppings $\tilde{t}_{xz}$ and $\tilde{t}_{x^2-y^2}$, and a crossed term $\tilde{t}_{x^2,x^2-y^2}$. To reduce the number of free parameters, we fix the hopping ratios to the values in the bulk, $\tilde{t}_{xz} : \tilde{t}_{x^2-y^2} : -\tilde{t}_{x^2,x^2-y^2} = t^{\text{bulk}}, t^{\text{bulk}} : t^{\text{bulk}}$. The minus sign in $\tilde{t}_{x^2,x^2-y^2}$ accounts for the $\pi/2$ rotation of the hopping direction with respect to $R_1$, which is the reference for the hopping amplitudes in the bulk [16]. Figure 2(d-f) shows the spectrum for increasing values of $|\tilde{t}_{x^2,x^2-y^2}| = 0.2, 0.6, 1.0$ eV. The results are very similar to those obtained with the single-hopping model. Allowing for hoppings involving the $d_{xy}$-orbital does not change significantly the results, which agrees with $d_{xy}$ minor role in TGB states.

In both models we allowed for hopping values $t \sim 1$ eV. These are higher then bulk values [16], consequence of the shorter NN distance between M-atoms on opposite sides of the TGB. We have deliberately ignored spin-orbit coupling (SOC) since TGB states derive from the X-edge states, which are weakly affected by SOC. Intrinsic spin-orbit coupling can be easily incorporated [25–27], but only at very low temperatures will the spin-degeneracy assumption break down.

\textit{Continuum theory and topological considerations}.—A continuum theory describing the left ($y < 0$) and right ($y > 0$) regions [see Fig. 1(a)] can be derived from the three-orbital TB model (see Supplemental Material). The Hamiltonian reads

$$\mathcal{H}_\mu(q) = v_0(q) \sigma_z + \mu_0 \sigma_y + (\Delta + \beta q^2) \sigma_z + \epsilon_F \sigma_0,$$

where $q = \mathbf{k} - \mathbf{\tau K}$ is the small wave vector with respect to valley $K$ ($\tau = +1$) or $K'$ ($\tau = -1$), $\mu = +1$ on the left ($y < 0$) and $\mu = -1$ on the right ($y > 0$) regions, and $\epsilon_F$ is the chemical potential. The Pauli matrices $\sigma_i = x,y,z$ act on the space of conduction and valence band states at $\tau K$, with $\sigma_0$ for the identity. For MoSe$_2$, the coefficients take the values: $v_0 \simeq 5.6 \times 10^5$ ms$^{-1}$, $2\Delta \simeq 1.44$ eV, $\beta \simeq -3.01$ eV Å$^2$, and $\epsilon_F \simeq 0.76$ eV. Apart from SOC, we are ignoring electron-hole asymmetry and trigonal warp-
ing terms, which have much smaller coefficients (see Supplemental Material).

Equation (2) can be cast in the form \( \mathcal{H}_{\tau\mu}(q) = h(q) \cdot \sigma + e_F \sigma_0 \), where \( \sigma \) is the vector of Pauli matrices. The valley Chern number defined by \( C^v_{\tau\mu} = \frac{1}{2\pi} \int_{-\infty}^{\infty} \Omega^v_{\tau\mu}(q) dq_x dq_y \), with \( \Omega^v_{\tau\mu} \) the Berry curvature for the lower band [28, 29].

\[
\Omega^v_{\tau\mu}(q) = \frac{1}{2} \frac{\partial h}{\partial q_x} \times \frac{\partial h}{\partial q_y} \cdot \frac{h}{|h|^2}.
\]

After integration [30], we obtain

\[
C^v_{\tau\mu} = \frac{1}{2} \tau \mu \left[ \text{sign}(\Delta) - \text{sign}(\beta) \right].
\]

The dependence on \( \Delta \) and \( \beta \) is known [31, 32]: for \( \Delta > 0 \) and \( \beta < 0 \), the case of TMDs, the system is topologically non-trivial with \( C^v_{\tau\mu} = \tau \mu \). The dependence on \( \mu \), which accounts for the position, left or right, with respect to the TGB is new and needs clarification.

For a Chern number change \( \Delta C^v_{\tau\mu} = |C^v_{\tau\mu+1} - C^v_{\tau\mu-1}| = 2 \), we would expect two chiral modes per valley (per spin) running along the boundary, as implied by the bulk-edge correspondence [19]. These modes appear as bound states of the Hamiltonian \( \mathcal{H}_{\tau\mu}(q_x, y) \), obtained from Eq. (2) with \( q_y = -i \partial_y \) and \( \mu = \mu(y) \), where \( \mu(y < 0) = +1 \) and \( \mu(y > 0) = -1 \). Close inspection shows that no bound state solution exists, contrary to other 2D systems with domain walls [33–35]. This is consistent with the absence of a gap closing associated with a change of sign in \( \mu \) (the spectrum \( E_q = e_F \pm |h(q)| \) is independent of \( \mu \)). The apparent discrepancy stems from the transformation \( y \to -y \) relating left and right regions, which implies a reversal of the chirality of edge states, and thus a sign change of the valley Chern number [36], but not a gap closing. The lack of topological protection is crucial to make our TB results compatible with experiments. Indeed, for a filling \( n = 2/3 \) (including spin), expected for the charge neutral system, a single 1D band – and not two – crossing the Fermi level was observed [4]. The stability of these states can be linked to the 1D Berry phase difference between the two sides of the TGB Zhu et al. [20] (see Supplemental Material).

Effect of correlations.—A decisive low-energy property of 1D metallic correlated systems is the low-energy power-law suppression of the density of states (SDS) at the Fermi level [2, 4, 37]. The experimental value of the corresponding power-law SDS exponent \( \alpha \) is typically larger than 1/2 [2, 4, 37]. One finds \( \alpha < 1/8 \) for the integrable 1D Hubbard model (1DHM) with onsite repulsion [4] and \( \alpha > 1/8 \) for lattice electronic systems with an interaction range larger than one lattice spacing [38]. Consistently with the robust 1D nature of the MoSe\(_2\) line defects found here, the studies of Ref. [4] have used a renormalized version of the 1D MQIM approach [3] to describe their ARPES peaks distribution. It relies on a transformation of the 1DHM pseudofermion dynamical theory (PDT) [39], which for integrable models is equivalent to the MQIM [3, 39], into a renormalized MQIM that accounts for the electronic finite-range interactions.

Such a transformation refers to gently turning on the finite-range part of the electronic potential \( V_e(r) \) where \( r \) is the electron distance. It maps the 1DHM parameter \( \xi_c = \sqrt{2K_c} \in [1, \sqrt{2}] \) onto \( \xi_c' = \sqrt{2K_c} \in [1/2, \xi_c] \). Here \( K_c \) and \( K_c' \) are corresponding TLL charge parameters [2, 4, 37, 38]. The 1DHM \( U \) becomes under the transformation an effective interaction \( U_{\text{eff}} = U \) such that \( U_{\text{eff}} \to U \) for \( \xi_c \to \xi_c' \) yet \( U_{\text{eff}} \neq U \) for \( \xi_c < \xi_c' \). Here \( U \) is the actual onsite repulsion in \( V_e(r) \) at \( r = 0 \) for the range \( \xi_c < \xi_c' \) for which the interaction \( U_{\text{eff}} \) has contributions from both onsite and finite-range interactions.

According to the principle of emergence, the properties of a physical system are mainly determined by how electrons are organized in it [40]. In the case of the correlated electronic systems to which the MQIM applies [3], such an organization gives rise to emerging fractionalized particles whose phase shifts are imposed by mobile quantum impurities created under transitions to excited states.

For the renormalized MQIM [4], the emerging particles are the charge \( c \) and spin \( s \) (or \( s1 \)) pseudofermions, respectively.

The one-electron removal spectral function in the \((k, \omega)\)-plane vicinity of three singular features called spin \( s \) branch line and charge \( c \) and \( c' \) branch lines, respectively, has the universal MQIM form \( \tilde{B}(k, \omega) \propto (\tilde{\omega}_+(k) - \omega)^{-\xi_\tau(k)} \) for small \( (\tilde{\omega}_+(k) - \omega) > 0 \). Here \( \tau = s, c, c' \), \( \omega < 0 \), and \( \tilde{\omega}_+(k) \) is the branch-line spectrum [4]. The \( \tau = s, c, c' \) branch lines refer actually to singular spectral features and thus ARPES peaks for the wave vector \( k \) ranges for which the exponents \( \xi_\tau(k) \) are negative. Their expressions involve \( c \) and \( s \) pseudofermion phase shifts imposed by mobile impurities [4]. On the one hand, the \( s \) pseudofermion phase shifts remain unrenormalized and due to the spin SU(2) symmetry are independent of the interaction. On the other hand, the phase shifts \( -2\pi \Phi_{c,\beta}(\pm k_F, q) \) imposed to \( c \) pseudofermions of momentum \( \pm k_F \) by creation of one charge \( (\beta = c) \) or spin \( \beta = s \) mobile impurity at \( \beta \) band momentum \( q \in [-q_{F\beta}, q_{F\beta}] \) under one-electron removal excitations are renormalized by the finite-range interactions [4]. Here \( q_{F\beta} = 2k_F, q_{F's} = k_F, \) and \( 2k_F = \pi n_c \) where \( n_c \) is the electronic density.

The renormalized MQIM applied provides that \( \lim_{r \to \infty} r V_e(r) = 0 \). In this case \( V_e(r) \) gives rise to an attractive potential \( V_c(x) \) associated with the interaction of the charge \( c \) pseudofermion and the charge mobile impurity at spatial distance \( x \) that vanishes for large \( x \) as \( V_c(x) = -C_c/x'. \) Here \( l \geq 6 \) is an integer determined by the large-\( r \) behavior of \( V_e(r), C_c = (2r_I)^{l-2}/\mu_I, r_I \) is a
length scale (van der Waals length for \( l = 6 \)), and \( \mu_l \) is the reduced mass. The renormalization of \(-2\pi \Phi_{c,c}(\pm 2k_F, q)\) and \(-2\pi \Phi_{c,s}(\pm 2k_F, q)\) involves the factors \( \xi_c^2 \) and \( \xi_s^2 \), respectively [4]. That of \(-2\pi \Phi_{e,c}(\pm 2k_F, q)\) involves the emergence of an additional term imposed by \( V_c(x) \) associated with an effective range \( R_{\text{eff}} \) that vanishes for the 1DHM. As in 3D two-body s-wave interactions (see Supplementary Materials), for small relative momentum \( k_r = (q \pm 2k_F) \) obeying the inequality \( |k_r| \ll (t/U_{\text{eff}}) \tan(\pi n_c) \) the 1DHM and renormalized phase shifts \(-2\pi \Phi_{e,c}(\pm 2k_F, q)\) have effective range expansions \( \cot(-2\pi \Phi_{e,c}(\pm 2k_F, q)) = -1/(a k_r) + \frac{1}{2} k_r R_{\text{eff}} \), respectively, whose higher terms are negligible. Here \( a \) and \( \bar{a} \) are the 1DHM and renormalized scattering lengths, respectively. The use of standard scattering theory for potentials with large-x behavior \( V_c(x) = -C_c/x^d \) where \( l \geq 6 \) [41] leads to \( R_{\text{eff}} = 1 - c_1 \left( \frac{a}{\bar{a}} \right)^2 + c_2 \left( \frac{a}{\bar{a}} \right)^4 \) in units of lattice spacing for the interval \( \xi_c \in [1/2, 1] \) for which \( \alpha > 1/8 \). Moreover, \( \frac{a}{\bar{a}} = \frac{\tan(\pi (\xi_c - 1)/\xi_c)}{\tan(\pi (\xi_c - 1)/\xi_c)} \) and \( c_1 \) and \( c_2 \) depend only on \( l \geq 6 \), decreasing from \( c_1 = c_2 = 2 \) at \( l = 6 \) to \( c_1 = 1 \) and \( c_2 = 1/3 \) in the \( l \to \infty \) limit [41].

In Ref. [4] it was considered that \( R_{\text{eff}} \approx 0 \) in the \( c, c \) phase-shift expression, which is acceptable provided that \( R_{\text{eff}} \approx 1 \) in units of lattice spacing. Here we confirm that such a condition holds for the MoSe\(_2\) line defects. Nevertheless, we show that accounting for the effects of \( R_{\text{eff}} \) improves the agreement with the experiments beyond that reached in Ref. [4]. As in that reference, the SDS exponent \( \alpha = (2 - \xi_c^2)^2/(8\xi_c^2) \) is chosen to refer to the \( \xi_c \) value for which there is agreement between the specific \( k \) intervals at which the \( \tau = s, c, c' \) branch-lines exponents \( \xi_{\tau}(k) \) are negative and the ARPES peaks distribution. For the \( s \) and \( c \) branch lines, these intervals are \( k \in [-k_F + \delta_{s,k}, k_F - \delta_{s,k}] \) and \( k \in [-2k_F + \delta_{c,k}, 2k_F - \delta_{c,k}] \), respectively. Here \( \delta_{s,k}/k_F \approx 0.12 \) and \( \delta_{c,k}/k_F \) is vanishing or very small. The \( c' \) branch line exponent should be positive for its whole \( k \) interval.

After suitable inclusion of \( R_{\text{eff}} \) in the spectral-function exponents expression, the parameters values that at electronic density \( n_e = 2/3 \) lead to agreement between the above intervals of the \( s, c, \) and \( c' \) branch lines (see Fig. S2 (a)) and the line defects ARPES peaks distribution are \( u_{\text{eff}} = U_{\text{eff}}/At = 0.18, \alpha = 0.72, \) and \( l = 8 \) for transfer integral \( t = 0.58 \) eV. The corresponding \( \tau = c, c', s \) exponents \( \xi_{\tau}(k) \) are plotted as a function of \( k \) in Fig. 3 for different \( \alpha \) values. The matching \( \alpha = 0.72 \) value refers to \( R_{\text{eff}} = 1.01 \) and agrees with the estimated experimental uncertainty, \( \alpha = 0.75 \pm 0.05 \) [4]. The prediction of Ref. [4] that \( \alpha = 0.78 \) for \( u_{\text{eff}} = 0.20 \) lays in that uncertainty range, which confirms that the approximation of using \( R_{\text{eff}} = 0 \) in the \( c, c \) phase shift expression is acceptable.

The room-temperature experimental SDS of the MoSe\(_2\) line defects is plotted in Fig. S3 along with analytical lines for \( \alpha = 0.70, 75, 80 \). The theoretical SDS power-law behavior in Fig. S3 though only applies at very low energy, up to \( \approx 0.07 \) eV. Comparison with the experimental points for that energy range reveals that concerning the \( \alpha = 0.70, 75, 80 \) theoretical lines the best agreement is reached at \( \alpha = 0.70 \). This is consistent with our correction from \( \alpha = 0.78 \) to \( \alpha = 0.72 \) improving the agreement.

Conclusions.— Confined states at TGBs in MoSe\(_2\) were shown to be well described by a three orbital TB model, which is robust to the details of the defect hoppings. The presence of a single band (per spin) at the Fermi level is consistent with experiments. Modeling the confined states as a 1D interacting electronic system unveils a MQIM (\( k, \omega \))-plane behavior with an effective range for the charge fractionalized particle - charge mobile impurity interaction that extends up to the lattice spacing, in excellent agreement with ARPES measurements. The robustness and the properties found here for 1D confined states in MoSe\(_2\) extend to the full semiconducting TMD family, giving rise to a new paradigm where one-dimensionality is protected by the two-dimensionality of the host material.

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Supplementary Materials: Robust one-dimensionality at twin-grain-boundaries in MoSe₂

I. DERIVATION OF THE CONTINUUM THEORY

Consider the 3-band tight-binding Hamiltonian of TMDs, given by [S1]

$$\mathcal{H} = \sum_k \hat{\psi}_k^\dagger H(k) \hat{\psi}_k,$$

(S1)

with $\hat{\psi}_k^\dagger = (\hat{c}_{x_1}^\dagger, \hat{c}_{x_2}^\dagger, \hat{c}_{x_3}^\dagger, \hat{c}_{x'-y_2}^\dagger)$, and

$$H(k) = \begin{pmatrix} h_0 & h_1 & h_2 \\ h_1^* & h_{11} & h_{12} \\ h_2^* & h_{12} & h_{22} \end{pmatrix},$$

(S2)

where

$$\begin{align*}
h_0 &= \epsilon_1 + 2t_0 \cos 2\alpha + 4t_0 \cos \alpha \cos \beta \\
h_{11} &= \epsilon_2 + 2t_{11} \cos 2\alpha + (t_{11} + 3t_{22}) \cos \alpha \cos \beta \\
h_{22} &= \epsilon_2 + 2t_{22} \cos 2\alpha + (t_{22} + 3t_{11}) \cos \alpha \cos \beta \\
h_1 &= 2it_1 \sin 2\alpha + 2it_1 \sin \alpha \cos \beta - 2\sqrt{3}t_2 \sin \alpha \sin \beta \\
h_2 &= 2t_2 \cos 2\alpha - 2t_2 \cos \alpha \cos \beta + 2\sqrt{3}it_1 \cos \alpha \sin \beta \\
h_{12} &= 2it_{12} \sin 2\alpha - 4it_{12} \sin \alpha \cos \beta + \sqrt{3}(t_{22} - t_{11}) \sin \alpha \sin \beta,
\end{align*}$$

(S3)

$$\alpha = k_x a/2, \quad \beta = \sqrt{3}k_y a/2.$$ The two $\mathcal{K}$-points in the BZ are

$$\tau \mathcal{K} = (\tau \frac{4\pi}{3a}, 0),$$

(S4)

which gives $\alpha_{\pm} = \pm \frac{2\pi}{3}, \beta_{\pm} = 0$.

The Taylor expansion to the second order, near the $\mathcal{K}$-points, reads:

$$H(\tau \mathcal{K} + \mathbf{q}) = H(\tau \mathcal{K}) + H^{(1)}_{\mathbf{q}} + H^{(2)}_{\mathbf{q}} + \mathcal{O}(aq)^3$$

$$= H(\tau \mathcal{K}) + q_i(\partial_i H)\tau \mathcal{K} + \frac{1}{2} q_i q_j(\partial_i \partial_j H)\tau \mathcal{K} + \mathcal{O}(aq)^3$$

(S5)

$$= \begin{pmatrix} \eta_0 & \eta_1 & \eta_2 \\ \eta_1^* & \eta_{11} & \eta_{12} \\ \eta_2^* & \eta_{12}^* & \eta_{22} \end{pmatrix} + a \begin{pmatrix} u_0 & u_1 & u_2 \\ u_1^* & u_{11} & u_{12} \\ u_2^* & u_{12}^* & u_{22} \end{pmatrix} + a^2 \begin{pmatrix} v_0 & v_1 & v_2 \\ v_1^* & v_{11} & v_{12} \\ v_2^* & v_{12}^* & v_{22} \end{pmatrix} + \mathcal{O}(aq)^3,$$

(S6)

with

$$\eta_0 = \epsilon_1 - 3t_0, \quad \eta_{11} = \epsilon_2 - \frac{1}{2}(3t_{11} + 3t_{22}), \quad \eta_{22} = \epsilon_2 - \frac{1}{2}(3t_{11} + 3t_{22}),$$

$$\eta_1 = 0, \quad \eta_2 = 0, \quad -ir\sqrt{3}t_{12},$$

(S7)

$$u_0 = 0, \quad u_{11} = \frac{3\sqrt{3}}{4} r(t_{11} - t_{22}) q_x, \quad u_{22} = \frac{3\sqrt{3}}{4} r(t_{22} - t_{11}) q_x,$$

$$u_1 = -\frac{3}{2} t_1 q_x - r\frac{3\sqrt{3}}{2} t_2 q_y, \quad u_2 = r\frac{3\sqrt{3}}{2} t_2 q_x - \frac{3}{2} t_1 q_y, \quad u_{12} = \frac{3\sqrt{3}}{2} (t_{22} - t_{11}) q_y,$$

(S8)

and

$$v_0 = \frac{3}{4} t_0 q_x^2, \quad v_{11} = \frac{3}{16} [(3t_{11} + t_{22}) q_x^2 + (t_{11} + 3t_{22}) q_y^2], \quad v_{22} = \frac{3}{16} [(t_{11} + 3t_{22}) q_x^2 + (3t_{11} + t_{22}) q_y^2],$$

$$v_1 = \frac{3}{4} t_2 q_x q_y + ir\frac{3\sqrt{3}}{8} t_1(q_x^2 - q_y^2), \quad v_2 = \frac{3}{8} t_2 (q_x^2 - q_y^2) - ir\frac{3\sqrt{3}}{4} t_1 q_x q_y, \quad v_{12} = \frac{3}{8} (t_{11} - t_{22}) q_x q_y + ir\frac{3\sqrt{3}}{4} t_{12} q^2.$$

(S9)
Diagonalizing the 0th order Hamiltonian,

\[ H(\tau K) = \begin{pmatrix} \epsilon_1 - 3t_0 & 0 & 0 \\ 0 & \epsilon_2 - \frac{1}{2}(3t_{11} + 3t_{22}) & -i\tau \sqrt{3}t_{12} \\ 0 & -i\tau \sqrt{3}t_{12} & \epsilon_2 - \frac{1}{2}(3t_{11} + 3t_{22}) \end{pmatrix}, \]  

(S10)

one obtains for the respective eigenvectors and eigenvalues

\[
|\psi^c(\tau K)| = |\psi^a(\tau K)|, \quad \epsilon_c = \epsilon_1 - 3t_0 \\
|\psi^v(\tau K)| = \frac{1}{\sqrt{2}} \left[ |\psi^c(\tau K)| + i|\psi^b(\tau K)| \right], \quad \epsilon_v = \epsilon_2 - \frac{1}{2}(3t_{11} + 3t_{22}) - 3\sqrt{3}t_{12} \\
|\psi^b(\tau K)| = \frac{1}{\sqrt{2}} \left[ |\psi^c(\tau K)| - i|\psi^b(\tau K)| \right], \quad \epsilon_h = \epsilon_2 - \frac{1}{2}(3t_{11} + 3t_{22}) + 3\sqrt{3}t_{12}.
\]  

(S11)

The transformation matrix that diagonalizes \( H(\tau K) \) reads

\[
U_{\tau} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -i\tau/\sqrt{2} & 1\tau/\sqrt{2} \\ 0 & i\tau/\sqrt{2} & 1\tau/\sqrt{2} \end{pmatrix},
\]

(S12)

and the first-order matrix in the eigenbasis of \( H(\tau K) \) is to be written as

\[
\Sigma^{(1)}(q) = U_{\tau} H^{(1)}(q) U_{\tau}^{-1} = \left( \begin{array}{ccc} u_0 & \frac{1}{\sqrt{2}}(u_2 + i\tau u_1) & \frac{1}{\sqrt{2}}(u_2 - i\tau u_1) \\ \frac{1}{\sqrt{2}}(u_2 + i\tau u_1)^* & \frac{1}{2}(u_{22} + u_{11}) + \tau \text{Im}[u_{12}] & \frac{1}{2}(u_{22} - u_{11}) - i\tau \text{Re}[u_{12}] \\ \frac{1}{\sqrt{2}}(u_2 - i\tau u_1)^* & \frac{1}{2}(u_{22} - u_{11}) + i\tau \text{Re}[u_{12}] & \frac{1}{2}(u_{22} + u_{11}) - \tau \text{Im}[u_{12}] \end{array} \right)
\]

\[
= a \left( \begin{array}{ccc} 0 & t^{(1)}_{vc}(\tau q_x - i\tau q_y) & t^{(1)}_{ch}(\tau q_x + i\tau q_y) \\ t^{(1)}_{vc}(\tau q_x + i\tau q_y) & 0 & t^{(1)}_{ch}(\tau q_x - i\tau q_y) \\ t^{(1)}_{ch}(\tau q_x - i\tau q_y) & t^{(1)}_{ch}(\tau q_x + i\tau q_y) & 0 \end{array} \right),
\]

(S13)

with

\[
t^{(1)}_{vc} = \frac{3}{2\sqrt{2}}(\sqrt{3}t_2 + t_1), \quad t^{(1)}_{ch} = \frac{3}{2\sqrt{2}}(\sqrt{3}t_2 - t_1), \quad t^{(1)}_{vh} = \frac{3 \sqrt{3}}{4}(t_{22} - t_{11}).
\]

(S14)

The second order correction to the Hamiltonian can be written as

\[
\Sigma^{(2)}(q) = U_{\tau} H^{(2)}(q) U_{\tau}^{-1} = a^2 \left( \begin{array}{ccc} v_0 & \frac{1}{\sqrt{2}}(v_2 + i\tau v_1) & \frac{1}{\sqrt{2}}(v_2 - i\tau v_1) \\ \frac{1}{\sqrt{2}}(v_2 + i\tau v_1)^* & \frac{1}{2}(v_{22} + v_{11}) + \tau \text{Im}[v_{12}] & \frac{1}{2}(v_{22} - v_{11}) - i\tau \text{Re}[v_{12}] \\ \frac{1}{\sqrt{2}}(v_2 - i\tau v_1)^* & \frac{1}{2}(v_{22} - v_{11}) + i\tau \text{Re}[v_{12}] & \frac{1}{2}(v_{22} + v_{11}) - \tau \text{Im}[v_{12}] \end{array} \right)
\]

\[
= a^2 \left( \begin{array}{ccc} \chi_c q_x^2 & t^{(2)}_{vc}(q_x - i\tau q_y)^2 & t^{(2)}_{ch}(q_x + i\tau q_y)^2 \\ t^{(2)}_{vc}(q_x + i\tau q_y)^2 & \chi_v q_y^2 & t^{(2)}_{vh}(q_x + i\tau q_y)^2 \\ t^{(2)}_{ch}(q_x - i\tau q_y)^2 & t^{(2)}_{vh}(q_x - i\tau q_y)^2 & \chi_h q_y^2 \end{array} \right),
\]

(S15)

with

\[
\chi_c = \frac{3}{4}t_0, \quad \chi_v = \frac{3}{8}(t_{11} + t_{22} + \sqrt{3}t_{12}), \quad \chi_h = \frac{3}{8}(t_{11} + t_{22} - \sqrt{3}t_{12}),
\]

\[
t^{(2)}_{vc} = \frac{3}{8\sqrt{2}}(t_2 - \sqrt{3}t_1), \quad t^{(2)}_{ch} = \frac{3}{8\sqrt{2}}(t_2 - \sqrt{3}t_1), \quad t^{(2)}_{vh} = \frac{3}{16}(t_{22} - t_{11}).
\]

(S16)

The effective second order Hamiltonian of the lowest conduction and highest valence bands is then given by

\[
H_{eff}(q) = P_L \left[ H_0 + \Sigma^{(1)}(q) + \Sigma^{(2)}(q) \right] P_L + \sum_{l=c,v} \frac{|\psi_l\rangle\langle\psi_l| \Sigma^{(1)}(q) P_L \Sigma^{(1)}(q) |\psi_l\rangle\langle\psi_l|}{\epsilon_l - \epsilon_h} + \sum_{m,n,m \neq c,v,n \neq c,v} \frac{|\psi_m\rangle\langle\psi_m| \Sigma^{(1)}(q) P_L \Sigma^{(1)}(q) |\psi_n\rangle\langle\psi_n|}{\epsilon_m - \epsilon_h}
\]
with \( P_l = |\psi_e\rangle \langle \psi_e| + |\psi_o\rangle \langle \psi_o|, P_h = |\psi_h\rangle \langle \psi_h|, \) and \( \epsilon_F = \frac{\epsilon_e + \epsilon_o}{2}. \) After straightforward manipulation, we obtain

\[
H_{\text{eff}}(\mathbf{q}) = \left( \begin{array}{cc}
\epsilon_c & 0 \\
0 & \epsilon_v 
\end{array} \right) + a t_{\text{ee}}^{(1)} \left( \begin{array}{cc}
\tau q_x - i q_y & 0 \\
0 & \tau q_x + i q_y 
\end{array} \right) + a^2 \left( \begin{array}{cc}
\chi_v q_x^2 & t_{\text{ee}}^{(2)} (q_x + i q_y)^2 \\
t_{\text{ee}}^{(2)} (q_x - i q_y)^2 & \chi_v q_x^2 
\end{array} \right) +
\] (S17)

where \( \xi_c = \frac{t_{\text{ee}}^{(1)}}{\epsilon_v - \epsilon_e}, \xi_v = \frac{t_{\text{ee}}^{(1)}}{\epsilon_v - \epsilon_e}, t_{\text{ee}} = \frac{t_{\text{ee}}^{(1)} \tau_{\text{ee}}^{(2)}}{\epsilon_v - \epsilon_e}, v = at_{\text{ee}}^{(1)}, \Delta = \frac{\epsilon_e - \epsilon_v}{2}, \delta \xi = \frac{\epsilon_e - \epsilon_v}{2} + \frac{\epsilon_v - \epsilon_e}{2}, \zeta = \frac{t_{\text{ee}}^{(2)} + t_{\text{ee}}^{(2)}}{\epsilon_v - \epsilon_e}, \) and \( \tau \to \tau_3. \) Apart from the constant and the electron-hole asymmetry terms proportional to \( \sigma_0, \) there is also a trigonal warping term proportional to \( \zeta, \) as well as the massive Dirac Hamiltonian with a quadratic term. Estimates for MoSe\(_2\) give \( [S1], v = 5.6 \times 10^3 \text{m/s}, \Delta = 1.44 \text{eV}, \delta \xi = -0.30 \text{eV}, \zeta = 9.4 \text{meV}, \) and \( \xi = 0.8 \text{meV}. \)

An analogous derivation with \( y \to -y \) results in the same Hamiltonian with \( q_y \to -q_y. \)

II. THE BERRY PHASE AND ITS TOPOLOGICAL RELATION TO THE STATE AT TGB

The state localized at the TGB is topologically originated at the difference of Berry phase across the boundary \([S2].\)

The X- and M-edge states localize at the boundary along \( x, \) therefore the system can be viewed as 1D lattice periodically modulated by a parameter \( k_x, \) and the edge states can be described by a Berry phase defined as

\[
\gamma(k_x) = i \oint dk_y \langle u_{k_x,k_y} | \partial_{k_y} | u_{k_x,k_y} \rangle = \pi,
\] (S19)

with \( u_{k_x,k_y} \) the occupied state at 1/3 filling (without spin), obtained by diagonalizing Eq. \((S2) [S3].\) A topologically nontrivial 1D insulating system is generally characterized by a \( \tau \) Berry phase, and has a pair of topologically protected degenerate edge states localized at the two ends of the 1D chain. However, the X- and M-edge states of TMDs have different energy dispersions versus \( k_x, \) and \( \gamma(k_x) \) also varies continuously.

In Fig. S1 we illustrate the spectrum as a function of \( k_x \) under open boundary condition along \( y, \) and the corresponding Berry phase \( \gamma(k_x). \) The two edge states in Fig. S1(a) become degenerate at two certain values of \( k_x = k_{x,0} \) (and \( k'_{x,0} \)), corresponding to a Berry phase \( \gamma(k_{x,0}) = \pi. \) The Berry phase varies continuously away from \( k_{x,0}, \) thus the
Figure S2: (a) Raw ARPES data image of MoSe$_2$ line defects with energy versus wave vector ($k_f$) along the $\Gamma\Omega\Gamma$ direction in the Brillouin zone plus the theoretical $c$, $c'$, and $s$ branch-lines spectra.\cite{S6} for $u_{\text{eff}} = U_{\text{eff}}/4t = 0.18$, transfer integral $t = 0.58$ eV, and electronic density $n_e = 2/3$. The full and dashed lines refer to momentum ranges with negative and positive exponents, respectively. (b) Second-derivative ARPES images. Source: The experimental ARPES data are from Ref. \cite{S6}.

degeneracy of edge states is lifted. Nevertheless, the edge states can be interpreted as a continuation of the degenerate edge states at $k_{x,0}$, and thus topologically originated at the $\pi$ Berry phase. In the system with TGB that we consider in this work, the two sides of $y < 0$ and $y > 0$ correspond to the Berry phase $\gamma(k_x)$ and $-\gamma(k_x)$ respectively, and the state localized at the TGB can be associated with the difference of the Berry phase across the TGB \cite{S2}.

III. EFFECTIVE-RANGE EXPANSIONS IN 3D AND 1D

In three (spatial) dimensions (3D), the two-body s-wave interaction dominates at low densities and can be described by the effective range $r_e$ expansion,\cite{S4, S5} $\cot \delta_{c,c} = -\frac{1}{k_{c,a}} + \frac{1}{2} r_c k_c + O(k_c^2)$, first derived by Bethe \cite{S4} and Blatt and Jackson \cite{S5}. Here $a$ is the scattering length and $k_c$ the relative momentum. For the 3D s-wave interaction, the phase shift depends only on the absolute value $|k_c|$. In contrast, in the present 1D case the charge-charge phase shift $-2\pi \Phi_{c,c}(\pm 2k_F, q)$ is for small relative momentum $k_c = (q \pm 2k_F)$ an odd function of $k_c$ with the universal behavior $\cot(-2\pi \Phi_{c,c}(\pm 2k_F, q)) = -1/(\tilde{a} k_c) + 1/2 k_c + R_{\text{eff}}$ for the renormalized theory and $\cot(-2\pi \Phi_{c,c}(\pm 2k_F, q)) = -1/(a k_c)$ for the 1D Hubbard model (1DHM). Here $\tilde{a}$ and $a$ are the scattering lengths and $R_{\text{eff}}$ is the renormalized-theory $c$ pseudofermion - mobile impurity interaction effective range. As in the case of 3D s-wave scattering \cite{S4, S5}, the third and higher terms in the effective range expansion are negligible. For electronic densities in the interval $n_e \in [0, 1]$, that expansion only applies provided that $|k_c| \ll \frac{1}{U_{\text{eff}}} \tan(\pi n_e)$ \cite{S7}. Hence it does not apply (i) at and near electronic densities $n_e = 0$ and $n_e = 1$ and (ii) for any $0 < n_e < 1$ and very large $u_{\text{eff}} = U_{\text{eff}}/4t$.

IV. ARPES AND THEORETICAL IMAGES AND SDS EXPONENT

Except for suitable inclusion of the effective range $R_{\text{eff}}$ in the expression of the phase shift $-2\pi \Phi_{c,c}(\pm 2k_F, q)$, all quantities are defined as in Ref. \cite{S6}. The renormalized-MQIM $s$, $c$, and $c'$ branch-line spectra are plotted in Fig. S2 (a) as a function of the wave vector $k$ for $u_{\text{eff}} = 0.18$, transfer integral $t = 0.58$ eV, and electronic density $n_e = 2/3$. The raw ARPES data image of MoSe$_2$ line defects and corresponding second-derivative ARPES images are plotted in Figs. S2 (a) and (b), respectively.

Figure S3 displays the suppression of the density of states (SDS) of MoSe$_2$ line defects close to the Fermi-level measured at room temperature (to avoid charge-density wave transition) and corresponding analytical lines for SDS power-law exponent $\alpha = 0.70, \alpha = 0.75$, and $\alpha = 0.80$. The theoretical predicted SDS universal power-law behavior controlled by the exponent $\alpha = (2 - \xi_c^2)/(8\xi_c^2)$ only applies though at low energy estimated in the case of the data in Fig. S3 to be up to $\approx 0.07$ eV. For larger energy values the SDS loses its universal power-law behavior, its form becoming different and specific to each many-electron problem.
Figure S3: The suppression of the density of states of mirror twin grain boundaries in monolayer MoSe$_2$ close to the Fermi-level measured at room temperature and corresponding theoretical predicted power-law lines for $\alpha = 0.70$, $\alpha = 0.75$, and $\alpha = 0.80$. It is obtained by plotting the angle integrated photoemission intensity as a function of binding energy $\omega$. The experimental data are well fit for $\alpha = 0.75 \pm 0.5$ and thus with a corresponding uncertainty estimated to be as large as $\pm 0.05$. Source: Fig. 4(c) of Ref. [S6].

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