Topological invariants to characterize universality of boundary charge in one-dimensional insulators beyond symmetry constraints

Mikhail Pletyukhov,1 Dante M. Kennes,2 Jelena Klinovaja,3 Daniel Loss,3 and Herbert Schoeller1,

1 Institut für Theorie der Statistischen Physik, RWTH Aachen, 52056 Aachen, Germany and JARA - Fundamentals of Future Information Technology
2 Dahlem Center for Complex Quantum Systems and Fachbereich Physik, Freie Universität Berlin, 14195 Berlin, Germany
3 Department of Physics, University of Basel, Klingelbergstrasse 82, CH-4056 Basel, Switzerland

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In the absence of any symmetry constraints we address universal properties of the boundary charge \( Q_B \) for a wide class of tight-binding models with non-degenerate bands in one dimension. We provide a precise formulation of the bulk-boundary correspondence by splitting \( Q_B \) via a gauge invariant decomposition in a Friedel, polarization, and edge part. We reveal the topological nature of \( Q_B \) by proving the quantization of a topological index \( I = \Delta Q_B - \bar{\rho} \), where \( \Delta Q_B \) is the change of \( Q_B \) when shifting the lattice by one site towards a boundary and \( \bar{\rho} \) is the average charge per site. For a single band we find this index to be given by the winding number of the fundamental phase difference of the Bloch wave function between two adjacent sites. For a given chemical potential we establish a central topological constraint \( I \in \{-1,0\} \) related to charge conservation and particle-hole duality. Our results are shown to be stable against disorder and we propose generalizations to multi-channel and interacting systems.

Introduction— Motivated by the discovery of the Quantum Hall effect [1,2], the search for materials with topological edge states (TESs) has become a very important field of condensed matter physics and quantum optics [3-9], see Refs. [10-14] for reviews and textbooks. Routinely, topological insulators are classified via their symmetry class and dimension [15-24]. Topological invariants like Chern and winding numbers are established and can be used to predict TESSs at the boundary of two materials with different topological indices. Recently, the classification has been extended to include inversion symmetry within the field of topological crystalline insulators (TCIs) [25-30]. Here, the Zak phase [31] is the topological invariant which, via the so-called modern theory of polarization [32-36], can be related to the boundary charge \( Q_B \) [37-38]. However, since the Zak phase of an individual band is not gauge invariant an unknown integer of topological nature occurs in \( Q_B \). Away from symmetry restrictions, finite one-dimensional (1D) tight-binding models with a sinusoidal on-site potential were studied [39,40], where a continuous phase variable \( \varphi \) controls the offset of the potential. Surprisingly, in the long wavelength limit, \( Q_B(\varphi) \) reveals a universal linear slope which was shown to be stable against disorder and to be related to the quantized Hall conductance. The linear behavior can be explained from classical charge conservation which, however, leaves again an unknown integer undetermined. Shifting the lattice adiabatically by one site towards a boundary of a half-infinite system, the boundary charge changes by the constant amount \( \Delta Q_B = \bar{\rho} \), where \( \bar{\rho} \) is the average charge per site. This is a generalization of charge pumping [41,42], where the lattice is shifted by a whole unit cell such that the charge \( \nu e \), given by the number \( \nu \) of occupied bands, is shifted into the boundary and balanced by a corresponding number of edge states leaving the band.

These works raise two important, fundamental issues that are intimately related: (i) the unknown integer in the boundary charge needs to be characterized and (ii) the topological nature of \( Q_B \) and the relevance of symmetries should be addressed. This letter solves both of these issues by introducing an alternative route to the modern theory of polarization via a gauge invariant decomposition (addressing (i)) of \( Q_B \) in three parts defined by the Friedel, polarization, and edge charge, providing a precise formulation of the bulk-boundary correspondence. Addressing (ii) within our framework we show that \( I = \Delta Q_B - \bar{\rho} \), an invariant defined via shifting the lattice by one site towards a boundary, is quantized even beyond symmetry constraints.

We advance the description of \( I \) in two central ways for a wide class of tight-binding models with non-degenerate bands in 1D. The first central result relates to \( Q_B^{(\alpha)} \) of a single band \( \alpha \) and states that \( I_\alpha = -w_\alpha \in \{0,\pm1\} \), where the quantized and gauge invariant winding number \( w_\alpha \) is defined in terms of the fundamental phase-difference of the Bloch wave function across two adjacent sites to the right and left of the boundary defining a half-infinite system. We stress that this winding number can be accessed experimentally via measuring the charge. Furthermore, we show that \( w_\alpha \) contains more information than the Chern number and is related to the Zak phase only in case of inversion symmetry. The second central result is obtained for the total invariant \( I \) for given chemical potential \( \mu \) in some gap. Here, we show that particle-hole (p-h) duality implies the topological constraint \( I \in \{0,-1\} \) enforcing a corresponding constraint for the phase-dependence of the edge states. All
of our results are demonstrated to be stable against random disorder (breaking translational invariance) and we propose generalizations to multi-channel and interacting systems.

In an accompanying article we derive the central result rigorously by studying directly the conditions for the appearance of edge states from a convenient analytic continuation of Bloch states. The agreement with our physically motivated presentation in this letter reveals the surprising result that edge states are not the driving force for the constraint but have to adjust to a certain choice of the phase-dependence of the model parameters to respect charge conservation and p-h duality.

Model— We start with a generic nearest-neighbor tight-binding model with translational invariance and one orbital per site on a half-infinite system, see Fig. 1 for a sketch of the system. The unit cells are labelled by \( n = 1, 2, \ldots \), the sites within a unit cell by \( j = 1, \ldots, Z \). The position of a site is characterized by the index \( m = Z(n-1) + j \equiv (n,j) \). We take generic on-site potentials \( v_n = v_{nj} = v_j \) and hoppings \( t_m = t_{nj} = t_j \) depending only on \( j \). The Hamiltonian is given by

\[
H = \sum_{n=1}^{\infty} \left\{ \bar{v}_n a_n^\dagger a_m - (i a_n^\dagger a_{m+1} + \text{h.c.}) \right\}.
\]

All \( t_j \) are chosen real since the phases can be gauged away by a unitary transformation. We consider zero temperature and use units \( \hbar = e = a = 1 \), where \( a \) denotes the lattice spacing.

To address the central issue of how the properties of the system depend on the definition of the boundary we introduce a phase variable \( 0 \leq \varphi < 2\pi \) controlling the continuous shift of the lattice towards the boundary via \( \gamma_{j+1} = \gamma_j + \varphi = \gamma_j + \frac{2\pi j}{Z} \), with \( \varphi = \nu, t \), such that a phase change by \( \frac{2\pi}{Z} \) corresponds to a shift of the boundary by one site. Generically, we take the form \( \gamma_j = V F_\nu(\varphi + 2\pi j/Z) \) and \( t_j = t + \delta F_\nu(\varphi + 2\pi j/Z) \), with \( F_\nu(\varphi) = F_\nu(\varphi + 2\pi) \sim O(1) \). For the special case of a single cosine modulation our model is equivalent to the well-known generalized Aubry-André-Harper models which play a central role in the study of topological insulators.

Definition and decomposition of boundary charge— In the insulating regime, the density \( \rho(m) = \rho(n,j) \) of a half-infinite system is expected to approach the bulk value \( \rho_{\text{bulk}}(j) = \lim_{m \to \infty} \rho(n,j) \) of the infinite system exponentially fast. We show in Ref. 23 that the corresponding decay length \( \xi \sim t/\Delta \), where \( t \) is the average hopping and \( \Delta \) denotes the gap. Following Ref. 39, we define the boundary charge as a macroscopic average \( Q_B = \sum_{m=1}^{\infty} [\rho(m) - \bar{\rho}] f(m) \) of the excess density modeling a charge measurement probe characterized by some envelope function \( f(m) \) decaying slowly from unity to zero compared to the scales \( Z \) and \( \xi \). Here, \( \bar{\rho} = \frac{1}{Z} \sum_{j=1}^{Z} \rho_{\text{bulk}}(j) \) denotes the average particle charge per site. Separating \( \rho(m) - \bar{\rho} = [\rho(m) - \rho_{\text{bulk}}(j)] + [(\rho_{\text{bulk}}(j) - \bar{\rho}) \right\), the first term of \( \rho_{\text{bulk}}(j) \) leads to \( \sum_{m=1}^{\infty} [\rho(m) - \rho_{\text{bulk}}(j)] \) of the form

\[
Q_B = \sum_{m=1}^{\infty} [\rho(m) - \rho_{\text{bulk}}(j)] f(m), \quad f(m) = f(Z(n-1) + j) \approx f(Zn) + f(Zn)(-Z + j).
\]

Using \( \bar{\rho} = \sum_{j=1}^{Z} \rho_{\text{bulk}}(j) - \bar{\rho} = 0 \), we get \( Q_B = -\frac{1}{Z} \sum_{j=1}^{Z} [\rho_{\text{bulk}}(j) - \bar{\rho}] \), describing the negative bulk dipole moment per unit cell, in analogy to the surface polarization charge of a dielectric medium. Finally, separating \( \rho(m) = \rho_{\text{bulk}}(m) + \rho_{\text{edge}}(m) \), we find the following gauge-invariant decomposition of the boundary charge

\[
Q_B = Q_F + Q_P + Q_E,
\]

where \( Q_F = \sum_{n=1}^{\infty} \rho_F(m) \) and \( Q_E \) is the number of edge states. Interestingly, the form \( Q_B = Q_F + Q_P \) suggests a bulk-boundary correspondence. \( Q_B - Q_E \) referring to the boundary, and \( Q_F + Q_P \) containing the bulk properties.

Bunch states and Zak phase— We now express \( Q_F \) and \( Q_P \) via the Bloch states of the infinite system. The bulk spectrum consists of \( Z \) non-degenerate bands \( \alpha = 1, \ldots, Z \) (numerated from bottom to top) with \( Z-1 \) gaps \( \nu = 1, \ldots, Z-1 \) in between. We assume that each gap remains open for all \( \varphi \); see Fig. 2 for an illustration of the \( \varphi \)-dependence of the band structure. If the chemical potential \( \mu = \mu_\nu \) is somewhere in gap \( \nu \), we get \( \bar{\rho} = \nu/Z \) and can split \( Q_F = \sum_{\nu=1}^{\nu} Q_F^{(\nu)} \) and \( Q_P = \sum_{\alpha=1}^{\alpha} Q_P^{(\alpha)} \) into the contributions of the occupied bands, where \( Q_F^{(\nu)} = \sum_{m=1}^{\nu} \rho_F^{(\nu)}(m) \) and \( Q_P^{(\alpha)} = \frac{1}{2} \sum_{j=1}^{\nu} \rho_{\text{bulk}}^{(\alpha)}(j) \Delta f(\nu) / 2 \). The densities \( \rho_{\text{bulk}}^{(\nu)}(m) = \int_{-\nu}^{\nu} d\chi_k |\chi_k^{(\nu)}(m)|^2 \) and \( \rho_{\text{bulk}}^{(\nu)}(j) = \int_{-\nu}^{\nu} d\chi_k |\chi_k^{(\nu)}(n,j)|^2 \) can be expressed by the eigenstates \( \psi_k^{(\nu)}(n,j) \) of the half-infinite and infinite system, respectively, where \( \psi_k^{(\nu)}(n,j) \) denotes the quasi-momentum. Using the Bloch form \( \psi_k^{(\nu)}(n,j) = \frac{1}{\sqrt{2\pi}} \chi_k^{(\nu)}(j) e^{ikn} \), we find \( |\psi_k^{(\nu)}(n,j)|^2 = \frac{1}{\sqrt{2\pi}} \chi_k^{(\nu)}(j) e^{ikn} \) and \( \Delta f(\nu) / 2 \). The normalized Bloch states with \( \chi_k^{(\nu)}(Z) \) chosen real in order to fulfill the boundary condition \( \psi_k^{(\nu)}(0,Z) = (\chi_k^{(\nu)}(Z) e^{ikn} \) are
0. Together with \( \chi_k^{(\alpha)} = \chi_{k+2\pi}^{(\alpha)} \) this fixes uniquely the gauge of the Bloch states. Using the eigenstates we finally express \( \rho_F^{(\alpha)}(n, j) = -\frac{1}{2\pi} \int_{-\pi}^{\pi} dk [\chi_k^{(\alpha)}(j)]^2 e^{2\pi i n k} \) and \( \rho_{\text{bulk}}^{(\alpha)}(j) = \frac{1}{2\pi} \int_{-\pi}^{\pi} dk |\chi_k^{(\alpha)}(j)|^2 \) via the Bloch states, providing the charges \( Q_{F}^{(\alpha)} \) and \( Q_{P}^{(\alpha)} \). Using recursion relations for \( \chi_k^{(\alpha)}(j) \), provided by the nearest-neighbor hopping Hamiltonian, we show in Ref. [45] that \( Q_{F}^{(\alpha)} = -\frac{2\pi}{Z} \) can be expressed via the Zak phase \( \delta = i \int_{-\pi}^{\pi} dk \sum_{\alpha} |\chi_k^{(\alpha)}(j)|^2 \frac{d}{dk} \chi_k^{(\alpha)}(j) \) introduced in Ref. [31].

Remarkably, this relation holds only exactly when the gauge of \( \chi_k^{(\alpha)} \) is chosen such that \( \chi_k^{(\alpha)}(Z) \) is real which is fundamentally related to the boundary condition. This was, to the best of our knowledge, not noticed previously where the relation was only established \( \text{mod}(1) \) [37, 38]. We emphasize that the proper gauge is an essential ingredient to fix the unknown integer of \( Q_B \) and to give Eq. (1) a precise meaning in terms of the bulk-boundary correspondence.

**Invariant of a single band**—We now address the central issue how the boundary charge changes when we change the phase by \( \frac{2\pi}{Z} \). We first analyze the boundary charge of a single band \( Q_B^{(\alpha)} = Q_F^{(\alpha)} + Q_P^{(\alpha)} \), with \( Q_F^{(\alpha)} = -\frac{2\pi}{Z} \). The change \( \Delta Q_B^{(\alpha)}(\varphi) = Q_B^{(\alpha)}(\varphi + \frac{2\pi}{Z}) - Q_B^{(\alpha)}(\varphi) \) can be calculated from the Bloch states \( \chi_k^{(\alpha)} \) at phase \( \varphi + \frac{2\pi}{Z} \) of the shifted system. In the gauge where \( \chi_k^{(\alpha)}(Z) \) is real, they are given by \( \chi_k^{(\alpha)}(j) = e^{-i\varphi} \chi_k^{(\alpha)}(1) \chi_k^{(\alpha)}(j+1) \) for \( j = 1, \ldots, Z-1 \) and \( \chi_k^{(\alpha)}(Z) = e^{-i\varphi} \chi_k^{(\alpha)}(1) \chi_k^{(\alpha)}(1) \), where \( \varphi \) is the phase of the complex number \( \chi_k^{(\alpha)}(1) \). With this result one can calculate \( Q_F^{(\alpha)} \) and \( Q_P^{(\alpha)} \) of the shifted system and finds \( \Delta Q_F^{(\alpha)} = \rho_{\text{bulk}}^{(\alpha)}(1) - w_\alpha \) and \( \Delta Q_P^{(\alpha)} = 1/Z - \rho_{\text{bulk}}^{(\alpha)}(1) \), where \( w_\alpha = w[\theta_k^{(\alpha)}] \) is the integer and gauge invariant winding number corresponding to the phase difference \( \theta_k^{(\alpha)} = \varphi_k^{(\alpha)}(1) + k \) of \( \psi_{k,\text{bulk}}(m) \) between \( m = 1 \) and \( m = 0 \), with \( w[\theta_k^{(\alpha)}] = \frac{1}{2\pi} \int_{-\pi}^{\pi} dk e^{-i\varphi} \frac{d}{dk} \varphi_k^{(\alpha)} \). Remarkably, both \( \Delta Q_F^{(\alpha)} \) and \( \Delta Q_P^{(\alpha)} \) are not universal and depend on \( \rho_{\text{bulk}}^{(\alpha)}(1) \). However, taking the sum we can define an integer and universal invariant \( I_\alpha \) for band \( \alpha \)

\[
I_\alpha(\varphi) = \Delta Q_B^{(\alpha)}(\varphi) - \frac{1}{Z} = -w_\alpha(\varphi). \tag{2}
\]

As shown below \( I_\alpha \in \{0, \pm 1\} \) can only take three possible values, see Fig. 3. Due to charge conservation \( Q_B^{(\alpha)} \) will jump by \( \mp 1 \) when an edge state enters/leaves the band at \( \varphi^{(\alpha)}_\pm \). Therefore, \( I_\alpha \) will jump by \( \mp 1 \) at

**Fig. 2.** Illustration of the band structure and of the phase-dependence of the edge states (blue color) connecting the bands for \( Z = 5, t = 1, V = 0.5, \delta t = 0.1 \), and \( F_\alpha(\varphi) \) defined via three random Fourier components for \( \gamma = v, t, \) see Supplemental Material [45] for the concrete parameters. The chemical potentials \( \mu_\alpha \) in gap \( \nu \) are indicated by dashed horizontal lines, for which \( Q_B \) is calculated in Fig. 3. To the right we state the total numbers \( M_\pm(\mu_\alpha) \) of edge states entering/leaving the system corresponding to the four chemical potentials \( \mu_\alpha \).

**Fig. 3.** Boundary charge \( Q_B \) and the invariant \( I \) as function of \( \varphi \) for a half-infinite system using the parameters of Fig. 2 for several \( \mu_\alpha \). We show \( Q_B + \nu/2 \) to offset the different curves. Up to a \( 2\pi/Z \)-periodic function, \( Q_B \) shows on average a linear slope with jumps at the positions where edge states move above/below \( \mu_\alpha \). As shown in the right inset, \( Q_F \) or \( Q_P \) alone do not show any linear behaviour. The invariant is always quantized to \( I \in \{-1, 0\} \). The dashed line is the invariant with additional staggered onsite-disorder drawn from a uniform distribution \((0, 0.05)\) for a very large finite system of \( 5 \times 10^5 \) lattice sites. In the lowest panel we show the invariant \( I_\alpha \) with \( \alpha = 2 \) for a single band. It can only take the values \( I_\alpha \in \{0, \pm 1\} \).
\( \varphi = \varphi^{(e)}(\varphi = \varphi^{(o)} - \frac{2\pi}{Z}) \). We conclude that \( \omega\alpha(\varphi) \) characterizes the value and the jumps of \( I_\alpha(\varphi) \) in the whole phase interval, whereas the Chern number \( C^{(\alpha)} \), which is known to be the number of leaving minus the number of entering edge states \( [2, 10, 13, 22] \), is a measure for the sum over all jumps of \( I_\alpha \) at the entering/leaving points \( \varphi^{(o)}_{\pm} \) of the edge states. Therefore, \( \omega\alpha \) contains much more information than \( C^{(\alpha)} \) and characterizes a different physical quantity. In the special case of inversion symmetry \( \delta \) more information than \( C^{(\alpha)} \), whereas the Chern number \( C \), which is an integer irrespective of any symmetry conditions. As we have seen during the derivation the polarization charge \( Q_P \) plays a very important role for this result. Only for chiral symmetry (all \( v_j = 0 \) and half-filling or in case of inversion symmetry we get \( Q_P = 0 \).

**Total invariant**—Next we discuss the change of the total boundary charge \( Q_B \) given by \( \Delta Q_B = \sum \Delta Q_B^{(o)} + \Delta Q_B^{(e)} = \sum \omega\alpha I_\alpha + \frac{\nu}{2} + \Delta Q_E \), where \( \Delta Q_E \) is the change of the number of occupied edge states. This yields the result that the total invariant

\[
I(\varphi, \mu_\nu) \equiv \Delta Q_B(\varphi, \mu_\nu) - \frac{\nu}{2} \tag{3}
\]

is an integer irrespective of any symmetry conditions. As we have seen during the derivation the polarization charge \( Q_P \) plays a very important role for this result. Only for chiral symmetry (all \( v_j = 0 \) and half-filling or in case of inversion symmetry we get \( Q_P = 0 \).

**Particle-hole duality**—We now present intuitive arguments why the invariant is integer and which values are possible. Using charge conservation on average the particle charge \( \rho \) will be moved into the boundary when the system is shifted by one site, leading to \( \Delta Q_B = \rho \). Using the Pauli principle we find from charge conservation for the holes that on average the hole charge \( \rho_\rho = \rho - 1 \) is moved into the boundary. Since the hole density is defined by \( \rho\rho(m) = \rho(m) - 1 \) the boundary charges for holes and particles are the same. Therefore, we obtain another value \( \Delta Q_B = \rho - 1 \) and conclude

\[
\Delta Q_B(\varphi, \mu_\nu) \in \{ \rho, \rho - 1 \} \Leftrightarrow I(\varphi, \mu_\nu) \in \{0, -1\}. \tag{4}
\]

This provides also the result \( I_\alpha \in \{0, \pm 1\} \) since \( I_\alpha(\varphi) \) is the difference of \( I(\varphi, \mu_\nu) \) when \( \mu_\nu \) is chosen as the top or bottom of band \( \alpha \). Which value occurs for a given phase depends crucially on the model parameters and can not be predicted in general. To derive this result we have disregarded that during the shift edge states can cross \( \mu_\nu \), so that \( \Delta Q_B(\varphi, \mu_\nu) \) could in principle hold only \( \mod(1) \). However, the occurrence of edge states during the shift is rather artificial and depends crucially on the choice of the phase-dependence on the interval \( [\varphi, \varphi + \frac{2\pi}{Z}] \) via \( F_\gamma(\varphi) \). Therefore, the edge states are not the physical reason why \( Q_B \) can only change according to Eq. \( \Delta Q_B \).

\[
\Delta Q_B(\varphi, \mu_\nu) \in \{ \rho, \rho - 1 \} \Leftrightarrow I(\varphi, \mu_\nu) \in \{0, -1\}. \tag{4}
\]

In Ref. \( 22 \) we show that, for given model parameters \( \nu_j, t_j \) at phase \( \varphi \) (and, correspondingly, at all phases shifted by \( \frac{2\pi}{Z} \)), the phase dependence can always be chosen in such a way that no edge state crosses \( \mu_\nu \) in the phase interval \( [\varphi, \varphi + \frac{2\pi}{Z}] \). Therefore, since \( \Delta Q_B(\varphi, \mu_\nu) \) depends only on the model parameters at \( \varphi \), we obtain the two values stated in Eq. \( \Delta Q_B \).
Our intuitive interpretation for the occurrence of the allowed values for $\Delta Q_B$ suggest the results to be also stable against weak interactions [51] similar to the stability of bound states [52]. Furthermore, via dimensional reduction, we expect our results to be also relevant to the understanding of universal features of $Q_B$ in higher dimensions. In the special case of half-filling gap closings can occur such that the average slope of the linear term $M_\nu = 0$. In this case Weyl physics occurs with interesting quantization of the boundary charge itself [49].

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M.P. and D.M.K. contributed equally to this work.

* Email: schoeller@physik.rwth-aachen.de

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See Supplemental Material, where the parameters used in Fig. 2 are listed.

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