Bulk-and-edge to corner correspondence

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We show that two-dimensional band insulators, with vanishing bulk polarization, obey bulk-and-edge to corner charge correspondence stating that the knowledge of the bulk and the two corresponding ribbon band structures uniquely determines the fractional part of the corner charge irrespective of the corner termination. Moreover, physical observables related to macroscopic charge density of a terminated crystal can be obtained by representing the crystal as collection of polarized edge regions with polarizations $\vec{P}_\alpha$, where the integer $\alpha$ enumerates the edges. We introduce a particular manner of cutting a crystal, dubbed “Wannier cut”, which allows us to compute $\vec{P}_\alpha$. We find that $\vec{P}_\alpha$ consists of two pieces: the bulk piece expressed via quadrupole tensor of the bulk Wannier functions’ charge density, and the edge piece corresponding to the Wannier edge polarization—the polarization of the edge subsystem obtained by Wannier cut. For a crystal with $n$ edges, out of $2n$ independent components of $\vec{P}_\alpha$, only $2n-1$ are independent of the choice of Wannier cut and correspond to physical observables: corner charges and edge dipoles.

I. INTRODUCTION

While the bulk description of solid-state materials is often available, the description close to material’s boundaries (termination) is often not accessible. For this reason, a particularly important role for the material science is played by bulk quantities—they depend only on the material’s bulk although they predict certain quantity that can be measured once a boundary is introduced. In other words, the sole existence of the bulk quantities requires some form of bulk-boundary correspondence. To name few examples, the bulk electrical polarization of an insulator predicts fractional part of the end charge1–5, the bulk orbital magnetization6,7 predicts persistent current circulating along the boundary, bulk geometric orbital magnetization8 predicts fractional part of the time-averaged edge current circulating along the boundary of a periodically, adiabatically driven insulator, and the bulk magnetoelectric polarizability of a three-dimensional insulator predicts the fractional part of the surface charge density resulting from application of an external magnetic field.9,10

In the recent years,11,12 the term bulk-boundary correspondence is almost exclusively used in the context of topological phenomena. In that more strict sense, the bulk-boundary correspondence assumes that the bulk quantity is topological invariant, hence, the boundary quantity is quantized. Notable examples include quantum (spin) Hall effect where the Chern number (Kane-Mele invariant13,14) predicts quantized (spin) Hall conductance,15–17, and $\mathbb{Z}_2$ invariant predicting quantized zero-energy conductance of Kitaev chain.18–20 In this work, such more strict correspondence is referred to as topological bulk-boundary correspondence.12,21–23 In certain cases bulk-boundary correspondence can be enriched by the attribute “topological” in the presence of certain symmetries: the bulk polarization and the fractional part of the end charge become quantized in the presence of inversion symmetry, the bulk geometric orbital magnetization and the fractional part of the time-averaged edge current are quantized in the presence of inversion or fourfold rotation symmetry,8 and similarly, the magnetoelectric polarizability and the associated boundary quantity are quantized in the presence of time-reversal or inversion symmetry.9 On the other hand, there is no symmetry that quantizes the bulk orbital magnetization. It may be of interest to ask a reverse question: in which cases a topological bulk-boundary correspondence can be extended to its unquantized version. This work deals with one example where such extension is not possible—the bulk quadrupole moment and the corner charge. Namely, in the presence of fourfold rotation symmetry, the bulk quadrupole moment is topological invariant and it predicts the quantized corner charge, whereas in the absence of this symmetry constraint it is not possible to predict the corner charge without specifying the edge termination.25 In this work we show that instead of bulk to boundary correspondence, a bulk-and-edge to corner correspondence can be formulated.

In 2015, Zhou, Rabe, and Vanderbilt26 proposed that for band insulators, the fractional part of the corner charge $Q_c$ can be computed from the knowledge of the bulk and the two corresponding ribbon band structures via the following relation

$$Q_c = P_{\alpha x}^{\text{edge}} + P_{\alpha y}^{\text{edge}} \mod e, \quad (1)$$

where $P_{\alpha x}^{\text{edge}}$ ($P_{\alpha y}^{\text{edge}}$) is $x$-component ($y$-component) of the edge polarization for the edge along $x$ ($y$) direction. These authors defined the edge polarization in terms of so-called maximally localized hybrid Wannier functions,27 and verified the relation (1) using two tight-binding models.26 One year later, in their pioneering work, Benalcazar, Bernevig and Hughes proposed the model24 that in the presence of fourfold rotation symmetry exhibits quantized corner charge that is given by topological invariant dubbed “bulk quadrupole moment” $q_{xy}$,$^9$

$$q_{xy} = Q_c - P_{\alpha x}^{\text{edge}} - P_{\alpha y}^{\text{edge}} \mod e, \quad (2)$$

with $P_{\alpha x}^{\text{edge}}$ defined in the same manner as in Eq. (1). The non-vanishing value of “$Q_c - P_{\alpha x}^{\text{edge}} - P_{\alpha y}^{\text{edge}}$” proves that previously proposed relation (1) cannot hold in general. Note that fourfold rotation symmetry forces the relation $P_{\alpha x}^{\text{edge}} = -P_{\alpha y}^{\text{edge}}$ to hold, hence $q_{xy} = Q_c \mod e$ which expresses topological bulk-boundary correspondence. Subsequent works29,30 by
two independent groups proposed that established topological
bulk-boundary correspondence (2) can be extended to its
unquantized form. Moreover, the expression was proposed
that was meant to predict the corner charge using bulk Hamil-
tonian as its sole input. These findings were supported by
calculations on several tight-binding models. Although the
authors provided counter-examples showing that the proposed expression does not hold
in general. It follows from relation (2), that in the absence of
fourfold rotation symmetry constraint, the edge polarizations
\( \vec{P}_\alpha \) and \( \vec{P}_\alpha' \) are independent, thus the corner charge can be
modified by changing the termination only.\(^8\)

In this work we consider two-dimensional band insulators
with well-defined corner charge, which is the case when not
only the bulk but also the boundary is gapped and the bulk
polarization vanishes. Figure 1 shows one example of a ter-
minated crystal, with the index \( \alpha \) enumerating the corners.
The two edges, along the lattice vectors \( \vec{e}_\alpha \) and \( \vec{e}_{\alpha+1} \) with
the corresponding unit normal vectors \( \vec{n}_\alpha \) and \( \vec{n}_{\alpha+1} \), meet at
the corner with the index \( \alpha \). The main result of this work is
finding that the physical observables related to macroscopic
charge density \( \rho_{\text{macro}} \) of a terminated crystal—corner charges
and edge dipoles—can be obtained by replacing the crystal
with collection of polarized edge regions with polarizations
\( \vec{P}_\alpha' \), see Fig. 1. The edge polarizations \( \vec{P}_\alpha' \) consist of two
pieces,

\[
\vec{P}_\alpha' = L_\alpha \vec{q} \cdot \vec{n}_\alpha / 2 + \vec{P}_\alpha, 
\]

with \( L_\alpha = |\vec{e}_\alpha| \) being the shortest repeated length along \( \vec{e}_\alpha \).

The result (3) turns bulk-boundary correspondence for elec-
trical polarization\(^2\) into bulk-and-edge to corner correspon-
dence

\[
Q^\alpha_c = \frac{L_{\alpha+1}}{A_{\text{cell}}} \vec{P}_{\alpha} \cdot \vec{n}_{\alpha+1} + \frac{L_\alpha}{A_{\text{cell}}} \vec{P}_{\alpha+1} \cdot \vec{n}_\alpha \mod \epsilon, 
\]

where \( A_{\text{cell}} = |\vec{e}_\alpha \times \vec{e}_{\alpha+1}| \) is the area of the unit-cell defined
by the corresponding corner. The corner charge \( Q^\alpha_c \) is
obtained by integrating the crystal’s macroscopic charge den-
sity \( \rho \) over the corner region \( \vec{x} \in \mathbb{R}_c \) defined by the lines
\( \vec{x} \cdot \vec{n}_\alpha = \text{const} \) and \( \vec{x} \cdot \vec{n}_{\alpha+1} = \text{const} \), see Sec. II B. The
obtained bulk-and-edge to corner charge correspondence has
the same form as the one proposed\(^2\) in Eq. (1), albeit with
different definition for the edge polarization. Finally, the edge
dipole density \( D^\alpha_{\text{edge}} \) for the edge along \( \vec{e}_\alpha \) is given by trans-
verse component of the edge polarization,

\[
D^\alpha_{\text{edge}} = - \frac{\epsilon}{A_{\text{cell}}} \int_{x_{\alpha}}^{x_{\alpha+1}} dx_\alpha \int d\vec{x}_{\alpha+1} \cdot \vec{n}_\alpha \rho 
\]

where \( (x_{\alpha}, x_{\alpha+1}) \) are reduced coordinates in \((\vec{e}_\alpha, \vec{e}_{\alpha+1})\)-
basis, \( x_\alpha \) lies in the middle of the edge along \( \vec{e}_\alpha \), and the
integration bounds for \( x_{\alpha+1} \)-coordinate are from the edge to
the bulk, see Sec. II B. For a crystal with \( n \) edges, Eqs. (4) and
(5) give \( 2n - 1 \) physical observables.

The remaining of the article is organized as follows. In
Sec. II, we review modern theory of electrical polarizations
and explain how macroscopic charge density is obtained from
microscopic one, since the macroscopic charge density is used
to define corner charges. Sec. III contains the main results of
our work, there we formulate and prove bulk-and-edge to cor-
ner charge correspondence and introduce the notion of Wan-
nier cut. Two simple tight-binding models that illustrate the
procedure described in Sec. II B can be found in Sec. IV. We
conclude in Sec. V.

II. PRELIMINARIES

We start by reviewing modern theory of electric polariza-
tion of band insulators and the corresponding bulk-boundary
correspondence.\(^2\) In Sec. II B, we discuss how to compute
corner charges and edge dipoles for a terminated crystal.
A. Modern theory of electric polarization. Bulk-boundary correspondence.

For purposes of this work, we will be interested in polarization of a ribbon. Consider a ribbon infinite in \( \vec{e}_1 \)-direction, with \( N_2 \) unit-cells in \( \vec{e}_2 \)-direction, where \( \vec{e}_1, \vec{e}_2 \) are lattice vectors, see Fig. 2a. We assume that the ribbon is described by gapped \((N N_2) \times (N N_2)\) Bloch Hamiltonian \( h_{k_1} \), where \( N \) is the number of sites per unit-cell. For each \( k_1 \)-point, denote the projector onto occupied Bloch wavefunctions \( |\psi_{nk_1}\rangle \) by \( P_{k_1} = \sum_{n=1}^{N} |\psi_{nk_1}\rangle \langle \psi_{nk_1}| \), where the integer \( N_{\text{occ}} \) is the number of the occupied states per unit-cell. For the definition of \( P_{k_1} \), the scalar product is assumed to be taken over the supercell only, i.e., \( P_{k_1} \) is \((N N_2) \times (N N_2)\) matrix and \( P_{k_1+2\pi} = P_{k_1} \). Modern theory of electric polarization states that the polarization \( \vec{P} \) of the ribbon is given by

\[
\vec{P} = \frac{e}{2\pi} \left( i \ln \det' \left[ \prod_{k_1} P_{k_1} \right] \vec{e}_1 - \int_{0}^{2\pi} dk_1 \text{Tr} \left[ \vec{x} P_{k_1} \right] \right),
\]

(6)

where \( \det' U \) denotes the product of non-zero eigenvalues of \( U \), and \( \vec{x} \) is the position operator. The polarization (6) depends on the choice of the origin \( \vec{x} = 0 \), which can be avoided if the above expression is modified to include the ionic contribution \( \langle \vec{x} \rangle_{\rho_{\text{ion}}} \), where \( \rho_{\text{ion}}(\vec{x}) \) is ionic charge density. The bulk-boundary correspondence states

\[
Q_e \mod e = L \vec{B} \cdot \vec{n} / |\vec{e} \times \vec{e}_1|,
\]

(7)

where \( \vec{n} \) is a unit vector, perpendicular to some lattice vector \( \vec{e} \), and \( L = |\vec{e}| \) is the shortest repeated length along the direction \( \vec{e} \). The end charge \( Q_e \) is defined as integral of the macroscopic charge density of the terminated ribbon \( \rho_{\text{macro}} \) over the end region defined by the line \( \vec{x} \cdot \vec{n} = x_0 \), where \( x_0 \) is chosen deep in the bulk where the supercell charge neutrality is fulfilled with required accuracy, see Fig. 2b for the case \( \vec{e} = \vec{e}_2 \). The macroscopic charge density \( \rho_{\text{macro}} \) is obtained from microscopic one \( \langle \rho(\vec{x}) \rangle \) by performing convolution\(^{31}\) in space with some broadening function \( g(\vec{x}) \). One common choice for broadening function \( g(\vec{x}) \) is Gaussian function, in which case one passes (discretized) microscopic charge density \( \rho(\vec{x}) \) through Gaussian filter to obtain \( \rho_{\text{macro}}(\vec{x}) \). This approach requires visual inspection to make sure that the width of the Gaussian is chosen large enough to ensure sufficiently accurate charge neutrality in the bulk. A more straightforward approach to obtain \( \rho_{\text{macro}}(\vec{x}) \) is to perform moving window average of \( \rho \), where the “window” is chosen to be the unit square in the reduced coordinates \( \{x_1, x_2\} \), which are the coordinates in \( (\vec{e}_1, \vec{e}_2) \)-basis.\(^{32,33}\) The result of such moving average\(^{32}\) is that the end charge \( Q_e \) is obtained by integrating the function \( f_1(x_1) \rho(\vec{x}) \) over the whole space, where \( f_1(x_1) \) is ramp function

\[
f_1(x_1) = \begin{cases} 
0 & x_1 < x_{01} \\
x_1 - x_{01} & x_{01} \leq x_1 \leq x_{01} + 1 \\
1 & \text{otherwise},
\end{cases}
\]

(9)

with \( x_{01} \) lying in the bulk, see Fig. 2b.

An alternative formulation of electric polarization is obtained by expressing the projector onto the occupied states of the ribbon \( \mathcal{P} \) as

\[
\mathcal{P} = \sum_{R_1} \mathcal{P}_{R_1} = \sum_{R_1, n} |w_{R_1, n}\rangle \langle w_{R_1, n}|,
\]

(10)

where \( |w_{R_1, n}\rangle \) are (non-unique) exponentially localized Wannier functions (WFs) and \( R_1 \) enumerates different supercells of the ribbon. When the ribbon is infinite (or under periodic boundary conditions), the shape of WFs is independent of \( R_1 \) due to translational symmetry. The polarization (6) can be expressed using WFs as

\[
\vec{P} = -\epsilon \text{Tr} \left[ \mathcal{P}_{R_1} \vec{x} \right] \mod e R_1 \vec{e}_1,
\]

(11)

which is independent of \( R_1 \).

B. Macroscopic charge density, corner charge and edge dipole

As discussed in the previous subsection, a non-vanishing polarization \( \vec{P} \) of the crystal induces edge charge density
The macroscopic charge density $\rho^{\text{macro}}(\vec{x})$ for $\vec{x}$ in the corner region. The corner is defined by the two edges with the lattice vectors $\vec{e}_\alpha$ and the unit normal vectors $\vec{n}_\alpha$, $\alpha = 1, 2$. When the edge dipole moments are present, the middle of the edge “$\alpha$” is charge neutral only after averaging over a “supercell” consisting of many unit-cells in $\vec{e}_\alpha$-direction, $\{1, 2\} = \{(2, 1)\}$. Integrating $\rho^{\text{macro}}$ over different corner regions $\mathcal{R}_c$, denoted by dashed lines $\vec{x} \cdot \vec{n}_\alpha = x_{\alpha 0}$ and the hatched region, results in different corner charge.

which makes it difficult to define corner charge. For this reason, we consider a two-dimensional insulating crystal with vanishing bulk polarization and under open boundary conditions (flake). We focus on the area around the corner where the two edges, with lattice vectors $\vec{e}_\alpha$ and the unit normal vectors $\vec{n}_\alpha$ ($\alpha = 1, 2$), meet, see Fig. 3. Under present assumptions, the macroscopic charge density $\rho^{\text{macro}}$ consists of corner charges and edge dipoles as shown in Fig. 3, although there is certain freedom in the definition of the corner charge. For example, we may define the corner charge as integral of the macroscopic charge density $\rho^{\text{macro}}$ over the corner region $\mathcal{R}_c$, defined by the lines $\vec{x} \cdot \vec{n}_\alpha = x_{\alpha 0}$ with the point $(x_{01}, x_{02})$ lying in the bulk, see Fig. 3. Another independent physical observable is edge dipole moment (density) $D_\text{edge} = -e(\vec{x})\rho^{\text{macro}} \cdot \vec{n}_\alpha / A_{\text{cell}}$ where the averaging is over the supercell consisting of unit-cells starting from the middle of the edge along $\vec{e}_\alpha$ towards the bulk. Non-vanishing edge dipole implies that the charge neutrality in the middle of the edge along $\vec{e}_\alpha$ is achieved only after averaging $\rho^{\text{macro}}$ over the supercell consisting of unit-cells along $\vec{e}_\alpha$-direction, with the notation $\{1, 2\} = \{(2, 1)\}$ (that we use throughout this manuscript). Despite the fact that different choices of the corner region $\mathcal{R}_c$ result in different values of the corner charge, in practice one always measures current which is given by change of the corresponding corner charges. Hence, for the two edges meeting at a corner, the macroscopic charge density defines three independent physical observables: two edge dipoles and one corner charge.

The choice of $\mathcal{R}_c$ mentioned in the previous paragraph is particularly convenient, since one can obtain $\rho^{\text{macro}}$ by performing moving window average of $\rho$ with the window being the unit square in the reduced coordinates of $(\vec{e}_1, \vec{e}_2)$-basis. Hence, the corner charge is obtained by multiplying $\rho(\vec{x})$ with the product $f_1(x_1)f_2(x_2)$ of rump functions (9) and integrating over the whole space. For different choices of the corner region we obtain $\rho^{\text{macro}}$ by passing $\rho$ through Gaussian filter, since it is not clear how to chose the window for the moving average. Alternatively, the corner charge can be estimated from the flake’s quadrupole moment tensor for large enough flake, see Sec. III C.

III. BULK-AND-EDGE TO CORNER CORRESPONDENCE

In this section we formulate and prove the correspondence between the corner charge and the bulk-and-edge. To this end we consider a flake with vanishing bulk polarization, see Sec. II B, and focus on the upper right-corner, where for the purpose of the following discussion we may assume that the remaining three corners lie at infinity. The two edges have the unit normal vectors $\vec{n}_\alpha$ and the lattice vectors $\vec{e}_\alpha$, $\alpha = 1, 2$, defining unit-cell area $A_{\text{cell}} = |\vec{e}_1 \times \vec{e}_2|$, see Fig. 4. We perform two cuts along the lines $\vec{x} \cdot \vec{n}_\alpha = x_{\alpha 0}$, where the point $(x_{01}, x_{02})$ lies in the bulk. These cuts divide the flake into four subsystems, see Fig. 4: the two half-infinite edges (dotted region), the corner (hatched region), and the remaining bulk region. The polarizations of the two edge subsystems are denoted by $P_{\text{edge}}$, which are defined by modern theory of electric polarization, see Sec. II and Eq. (6). Denoting the corner charge of the “bulk” subsystem by $\bar{Q}_c$ and using the bulk-edge correspondence (7), we express the flake’s corner charge $Q_c$ as

$$Q_c = \bar{Q}_c + Q_{e1} + Q_{e2}$$

$$= \bar{Q}_c + \frac{L_2}{A_{\text{cell}}} P_{\text{edge}} \cdot \vec{n}_2 + \frac{L_1}{A_{\text{cell}}} P_{\text{edge}} \cdot \vec{n}_1 \mod e,$$

(12)

where in the first line we used that the corner subsystem is charge neutral (more generally, it contains integer multiple of electron charge $e$). The above relation assumes that the cut does not generate a net current-flow through the bulk.

FIG. 4. A charge neutral flake with total bulk polarization zero. The flake is semi-infinite in both dimensions. Two cuts (wavy lines) along a charge neutral lines $\vec{x} \cdot \vec{n}_\alpha = x_{\alpha 0}$ (\vec{x} \cdot \vec{n}_\alpha = x_{\alpha 0}) split the flake into four subsystems: the two edges (dotted regions), the corner (hatched region) and the remaining bulk subsystem. The fractional part of the upper-right corner charge is given by Eq. (12). If the cuts are chosen to be Wannier cuts, the resulting polarization of the edge-subsystem is called Wannier edge polarization $P_{\text{edge}}$. 

FIG. 3. The macroscopic charge density $\rho^{\text{macro}}(\vec{x})$ for $\vec{x}$ in the corner region. The corner is defined by the two edges with the lattice vectors $\vec{e}_\alpha$ and the unit normal vectors $\vec{n}_\alpha$, $\alpha = 1, 2$. When the edge dipole moments are present, the middle of the edge “$\alpha$” is charge neutral only after averaging over a “supercell” consisting of many unit-cells in $\vec{e}_\alpha$-direction, $\{1, 2\} = \{(2, 1)\}$. Integrating $\rho^{\text{macro}}$ over different corner regions $\mathcal{R}_c$, denoted by dashed lines $\vec{x} \cdot \vec{n}_\alpha = x_{\alpha 0}$ and the hatched region, results in different corner charge.
While many cuts allow one to separate the corner charge $Q_c$ into the three pieces (12), we additionally require that $Q_c$ is a bulk quantity and $\bar{\mathbf{P}}_{\text{edge}}^\alpha$ are edge quantities. To be more precise, we require that $Q_c$ is computable in terms of the bulk band structure, and similarly $\bar{\mathbf{P}}_{\text{edge}}^\alpha$ should be computable from the ribbon band structure for the ribbon along $\bar{\mathbf{e}}_\alpha$. This property is not satisfied for the cuts considered in the literature: the sharp cut as in Ref. 10, or the cut obtained by selecting maximally localized hybrid WFs close to the corresponding edge as in Ref. 26. Below we introduce a family of cuts for which we prove that the resulting $Q_c$ is expressed in terms of quadrupole tensor of the charge density of the bulk Wannier functions, and call such cuts “Wannier cut”. Subsection III B details on how to perform a translationally invariant Wannier cut to obtain the occupied states of the edge subsystem that allows us to define Wannier edge polarization $\bar{\mathbf{P}}_{\text{edge}}^\alpha$. With these definitions, the relation (12) becomes bulk-and-edge to corner correspondence, see Sec. III C.

A. Wannier cut: Wannier functions as “shape cutter”

The starting point for the Wannier cutting procedure is choice of the bulk WFs, whose components are denoted by $\bar{\rho}_{Rn}(\bar{x})$. Assuming that WFs are assigned to their home unit-cell, the charge density of WFs $\rho_{WF}(\bar{x})$ reads

$$\rho_{WF}(\bar{x} - \bar{R}) = -e \sum x |\bar{\rho}_{Rn}(\bar{x}^\prime)|^2 \delta(\bar{x} - \bar{x}^\prime) + \rho_{\text{ion}}(\bar{x}),$$

where we included the ionic contribution $\rho_{\text{ion}}^R$ to the unit-cell at $\bar{R}$. The second moment of the above charge density defines the (bulk) quadrupole tensor density $\bar{q}$,

$$\bar{q} = \frac{1}{A_{\text{cell}}} \sum_{\alpha, \beta = 1, 2} \bar{q}_{\alpha \beta} \bar{e}_\alpha \otimes \bar{e}_\beta,$$

where “⊗” denotes tensor product, $\bar{e}_\alpha$ are two linearly independent lattice vectors defining the unit-cell with the area $A_{\text{cell}} = |\bar{e}_1 \times \bar{e}_2|$, and $\bar{q}_{\alpha \beta} = (x_{\alpha \beta})_{\rho_{WF}} = \int dx_1 dx_2 \rho_{WF}(x_1, x_2)x_{\alpha \beta}$.

We now go back to the flake from Fig. 4, and select the rectangle $\square$ in the reduced coordinates $(x_1, x_2)$ of the edge lattice vectors $\bar{e}_\alpha$. We define $\square$-subsystem that consists of the flake’s WFs with the center in $\square$, see Fig. 5. For a large rectangle $\square$ deep in the bulk, the $\square$-subsystem is obtained by tilting the rectangle with the bulk WFs. Hence, its charge density $\rho_{\square}(\bar{x})$ takes a simple form

$$\rho_{\square}(\bar{x}) = \sum_{\bar{R} \in \square} \rho_{WF}(\bar{x} - \bar{R}).$$

Since the zeroth and the first moment of $\rho_{WF}(\bar{x})$ vanish, see Eq. (11), we have that the quadrupole tensor density of the $\square$-subsystem is the same as $\bar{q}$,

$$\bar{q}_{\square} = \bar{q}.$$

The obtained $\square$-subsystem is taken to corresponds to the bulk subsystem of Fig. 4. We want to prove that the corner charge and the edge dipole of $\square$-subsystem, $\bar{Q}_c^\alpha$ and $\bar{D}_{\text{edge}}^\alpha$, are expressed in terms of the bulk quadrupole tensor $\bar{q}$. We define $\bar{Q}_c$ using the corner region $\mathcal{R}_c$ with boundaries $\bar{x} \cdot \bar{n}_\alpha = x_{\text{occ}}$, see Sec. II B and Fig. 5. For the case when all the lattice sites lie on the lattice itself (lattice without the basis), $\bar{Q}_c$ can be obtained by integrating the microscopic charge density $\rho_{\square}^\alpha$ over the region $\mathcal{R}_c$,

$$\bar{Q}_c = \sum_{\bar{R} \in \square} \left[ -\theta(-R_1)\rho_{WF} - \theta(-R_2)\rho_{WF} + \theta(-R_1)\theta(-R_2) \right.$$ \( + \theta(R_1)(\rho_{WF} - \theta(-R_2)) + \theta(R_2)(\rho_{WF} - \theta(-R_1)) \bigg] Q_{\bar{R}},$$

where we assume that the ionic charge contribution $eN_{\text{occ}}$ is also localized at the lattice sites and $R_{WF}$ is the radius of the WFs, see Fig. 5. In the above expression, the following notation was introduced,

$$\bar{Q}_{\bar{R}} \equiv \rho_{WF}(\bar{R}) = -e \sum_{n=1}^{N_{\text{occ}}} |w_{(0,0)n}(\bar{R})|^2 + eN_{\text{occ}} \delta_{B_1,0} \delta_{B_2,0},$$

and $\theta(x) = |x|H(x)$ with $H(x)$ being Heaviside step function. The three terms in the first line of the sum (17) count the charge contained in the region outside of $\mathcal{R}_c$ (not necessarily inside of $\square$), originating from the WFs with center in $\mathcal{R}_c$. Similarly, the second and the third line of the sum (17) correspond to the charge contained in $\mathcal{R}_c$, originating from the WFs with center in $\square \setminus \mathcal{R}_c$. Using the assumption that the bulk polarization vanishes \( \bar{P} = \sum_{\bar{R}} \bar{R}Q_{\bar{R}} = 0 \), we rewrite Eq (17) as,

$$\bar{Q}_c = \sum_{\bar{R} \in \square} R_1 R_2 \bar{Q}_{\bar{R}} = \frac{L_1 L_2}{A_{\text{cell}}} \bar{n}_1 \cdot \bar{n}_2,$$

where in the last equality we used Eq. (14), $L_\alpha = |\bar{e}_\alpha|$, and that the unit normal vectors $\bar{n}_\alpha$ point towards outside of the
subsystem. The above result is valid for both convex and concave angles $\angle(\mathbf{e}_1, \mathbf{e}_2)$. To obtain the edge dipole $\mathbf{D}_1^{\text{edge}}$ from the charge density $\rho_\square$, we consider a flake infinite in $\mathbf{e}_1$-direction (ribbon) and focus on the upper edge. For concreteness we assume that the unit-cells at the top edge of $\square$ have coordinates $(R_1, -1)$. Due to translational invariance the charge $\Omega_{R_2}$, defined as the charge contained within the unit-cell at $R_2$, is independent of $R_1$. Using Eqs. (15) and (18) we write,

$$\Omega_{R_2} = \sum_{R_2} R_2 Q_{R_2} = - \sum_{R_2 \geq 0} R_2 - \sum_{R_2 < 0} R_2,$$

(20)

where the notation $Q_{R_2} \equiv \sum_{R_1} Q_{R_2}$ has been used. The edge dipole, see Eq. (5), for the edge along $\mathbf{e}_1$ is expressed as

$$F_1^{\text{edge}} = \sum_{R_2} R_2 \Omega_{R_2} = - \sum_{R_2 \geq 0} R_2 - \sum_{R_2 < 0} R_2 = \frac{1}{2} \sum_{R_2} R_2^2 Q_{R_2},$$

(21)

Changing the order of the two sums in the above expression we obtain

$$\tilde{D}_1^{\text{edge}} = \sum_{R_2 \geq 0} R_2^2 Q_{R_2} - \sum_{R_2 < 0} R_2^2 Q_{R_2},$$

(22)

where the cutoff $R_{WF}$ drops out for the ribbon wider than the radius of the bulk WFs, and for writing the second line we used $\sum_{R_2} Q_{R_2} = \sum_{R_1} R_2^2 Q_{R_2} = 0$. Repeating the same calculation for the other edge, we can write

$$\tilde{D}_1^{\text{edge}} = \frac{L_2^2}{2A_{\text{cell}}} \mathbf{n}_\alpha \cdot \hat{q} \cdot \mathbf{n}_\alpha.$$

(23)

The obtained relations (19) and (23) show that the corner charge and the edge dipoles resulting from the microscopic average of the charge density $\rho_\square$, can be seen to be generated by polarizations $L_\alpha \cdot \hat{q} \cdot \mathbf{n}_\alpha / 2$, localized precisely long the four edges of $\square$. This result can be anticipated in light of relation (16) and “homogeneity” of the $\square$-subsystem. In the more general case, when the corner region $\mathcal{R}_c$ is defined by lines $\hat{x} \cdot \mathbf{n}_\alpha = x'_{\alpha 0}$, applying the bulk-boundary correspondence (7) to these edge polarizations gives

$$Q_c = \frac{L_1 |e_1' \times e_2'|}{|e_1' \times e_2'|} |n'_1 \cdot \hat{q} \cdot n_1 / 2 + \frac{|e_2'| L_2}{|e_1' \times e_2'|} |e_1' \cdot n'_2 \cdot \hat{q} \cdot n_2 / 2,$$

(24)

where $e_\alpha'$ are lattice vectors satisfying $e_\alpha' \cdot \mathbf{n}_\alpha = 0$, normalized such that $|e_\alpha'|$ gives the shortest repeated length in the lattice direction $e_\alpha$. The above expression reduces to Eq. (19) for $\mathbf{n}_\alpha = \mathbf{n}_\alpha$, achieving by considering a ribbon with the periodic boundary condition in $\mathbf{e}_\alpha$-direction. For concreteness we set $\alpha = 1$ and denote by $\mathcal{H}_k$, the Bloch Hamiltonian of the ribbon, with supercell having $2N_2 + 1$ unit-cells located at positions $R_2 \mathbf{e}_2$, $R_2 \in [-N_2, N_2]$. Translational invariant Wannier cut is performed using hybrid bulk WFs $|\tilde{w}_{k_1 R_{2n}}\rangle$,

$$|\tilde{w}_{k_1 R_{2n}}\rangle = \sum_{R_2 = -N_1}^{N_1} e^{i k_1 R_1} |\tilde{w}_{R_{2n}}\rangle,$$

(25)

where periodic boundary condition identifies the sites at $R_1 = -N_1$ with those at $R_1 = N_1$. The Wannier cut is performed in the middle of the ribbon supercell by removing $2L + 1$ hybrid bulk WFs $|\tilde{w}_{k_1 R_{2n}}\rangle$ with $R_2 \in [-L, L]$ from the space spanned by the occupied states

$$\mathcal{P}_{k_1}^{L} \equiv \mathcal{P}_{k_1} - \sum_{R_2 = -L}^{L} |\tilde{w}_{k_1 R_{2n}}\rangle \langle \tilde{w}_{k_1 R_{2n}}|.$$

(26)

The integer $L$ should be chosen sufficiently large such the projector $\mathcal{P}_{k_1}^{L}$ does not contain the sites from the middle unit-cell of the supercell, i.e.,

$$\mathcal{P}_{k_1}(\tilde{x}, \tilde{x}') \rightarrow 0,$$

(27)

for $x_2, x_2' \in [-1/2, 1/2]$. The more localized WFs are, the smaller the value of $L$ is required. The matrix elements of the projector onto occupied states of the edge subsystem above the Wannier cut read

$$\mathcal{P}_{k_1}^{\text{edge}}(\tilde{x}, \tilde{x}') = H(x_2) H(x_2') \mathcal{P}_{k_1}^{L}(\tilde{x}, \tilde{x'}).$$

(28)

Note that, for a ribbon with the fixed width $N_2$, the value of $L$ should not be too large, otherwise the hybrid bulk WFs do not fully belong to the space of occupied states of the ribbon. This can be diagnosed by inspecting the charge neutrality of the resulting edge subsystem’s supercell

$$\sum \int \frac{dk_1}{2\pi} \mathcal{P}_{k_1}^{\text{edge}}(\tilde{x}, \tilde{x}) \rightarrow N_{\text{occ}}(N_2 - L),$$

(29)

where the value on the right-hand side is the ionic charge—the removal of the hybrid bulk WF also removes the corresponding ionic charge. If the conditions (27) and (29) are satisfied with required accuracy, the Wannier cut has been performed successfully. The edge polarization $\tilde{P}_{1}^{\text{edge}}$ is given by Eq. (6) using $\mathcal{P}_{k_1}^{\text{edge}}$ in place of $\mathcal{P}_{k_1}$.

C. Discussion

Stitching together the bulk and the edge subsystems, we obtain the main result of our work, namely that the corner charges and the edge dipoles are determined by the edge polarizations (3). The bulk-and-edge to corner charge correspondence is obtained by substituting Eq. (24) and the expression for the edge polarization into Eq. (12)

$$Q_c = \frac{|e_1'|}{|e_2' \times e_1'|} \tilde{P}_1^{\text{edge}} \cdot n'_2 + \frac{|e_2'|}{|e_1' \times e_2'|} \tilde{P}_2^{\text{edge}} \cdot n'_1.$$

(30)
It is worth mentioning that not only Wannier polarization \( q^\text{edge} \) but also the edge polarization \( P^\text{edge} \) have four independent components whereas there are only three independent physical observables.

Let us now consider a crystal with inversion symmetric bulk. It is instructive to compare macroscopic charge density \( \rho \) with the origin at the center of the flake, which gives \( \langle x_1 x_2 \rangle \rho_{\text{flake}} \hat e_\alpha \otimes \hat e_\beta \). The above expression should be compared with Eq. (19), where now the whole inversion symmetric flake has \( N_1 \times N_2 \) unit-cells. The two lowest moments of the flake’s charge density \( \rho_{\text{flake}} \) vanish, and we write the second (quadrupole) moment as

\[
q_{\text{flake}} = \frac{1}{N_1 N_2 A_{\text{cell}}} \sum_{\alpha \beta} \langle x_1 x_2 \rangle \rho_{\text{flake}} \hat e_\alpha \otimes \hat e_\beta.
\]

The flake’s macroscopic charge density \( \rho_{\text{flake,macro}} \) consists of four corner charges \( Q_c \) with alternating signs superimposed with the edge dipoles. We denote the coordinates of the center-of-charge of the top-right corner by \( \bar{x} = \frac{1}{2} X_1 \hat e_1 + \frac{1}{2} X_2 \hat e_2 \) with the origin at the center of the flake, which gives \( \langle x_1 x_2 \rangle \rho_{\text{flake,macro}} = Q_c X_1 X_2 \). The corner charge \( Q_c \) can be approximated from the flake’s quadrupole moment as

\[
Q_c \sim \frac{X_1 X_2}{N_1 N_2} Q_c = \frac{L_1 L_2}{A_{\text{cell}}} \cdot \bar{n}_1 \cdot \bar{n}_2,
\]

since \( X_\alpha / N_\alpha \to 1 \) in the thermodynamic limit, \( N_\alpha \to \infty \). The above expression should be compared with Eq. (19), where the accuracy is exponentially increased as the size of \( \square \)-subsystem, obtained by tiling, is increased above the radius of the tile. On the other hand, the quality of the approximation of the corner charge by the flake’s quadrupole moment \( q_{\text{flake}} \) for a fixed flake’s size, depends strongly on boundary conditions which affect \( \bar{x} \). The relation (4) holds whenever the corner charge is well defined.

### IV. EXAMPLES

In this section we consider two two-dimensional tight-binding models which we use to illustrate the procedure described in the previous section. For each example, we perform two independent calculations: 1) diagonalizing the flake’s Hamiltonian, we obtain macroscopic charge density \( \rho_{\text{macro}} \), and subsequently the corner charge \( Q_c \) and the edge dipole \( D^\text{edge} \), and 2) we make a choice of the occupied bulk WF, calculate the bulk quadrupole tensor and the Wannier edge polarizations for the each edge of interest—these quantities give the edge polarization (3) that are used to compute the corner charge and the edge dipole moments, see Eqs. (4) and (5).

Alternatively, \( D^\text{edge}_\alpha \) can be obtained from the corresponding ribbon calculation. For the first example we consider corners with different orientations of the edges. The second example is meant to illustrate a scenario where the bulk contribution to the edge polarization (3) is small, which explains why it was overlooked in Ref. 26.

To carry out the above-mentioned calculations, we need to specify the bulk Hamiltonian and the edge boundary conditions. We consider a special form of boundary conditions that we call “theorist” boundary conditions: the Hamiltonian around the boundaries is assumed to be the same as the bulk Hamiltonian with the hoppings to the missing sites set to zero. Theorist boundary conditions are used here out of convenience, they do not have any particular relevance for realistic systems.

#### A. Orbitals without internal quadrupole moment

This example considers two-dimensional tight-binding model with two sites per unit-cell, defined on an arbitrary Bravais lattice with primitive vectors \( \vec{a}_1 \) and \( \vec{a}_2 \). The Hamiltonian is written as

\[
h = \sum_{\vec{R}} \left[ \sum_{\alpha=1,2} \left( (-1)^\alpha \delta |\vec{R}\alpha\rangle \langle \vec{R}\alpha| \right) + \sum_{d=1,2} \left( (-1)^d t |\vec{R}+\vec{a}_d\alpha\rangle \langle \vec{R}+\vec{a}_d\alpha| \right) \right],
\]

where \( |\vec{R}\alpha\rangle \) is the \( \alpha \)-orbital at the position \( \vec{R} \). The above Hamiltonian has inversion symmetry that maps \( \alpha \)-orbital into itself, hence the bulk polarization is quantized. We make a choice of parameters of Hamiltonian (33) such that the bulk is gapped at half filling and for theorist boundary conditions the corner charge is sizable, \( \delta = -1 \), \( t = -0.08 \), \( t_1 = 3.5 \times t \), and \( t_2 = -1.5 \times t \). It is easy to see that for these parameters, the bulk polarization vanishes.

The occupied bulk WF \( |\vec{w}_{\vec{R}}\rangle \) is chosen as follows. When all the hoppings are switched off \( t = 0 \), the maximally localized WF takes the form \( |\vec{w}_0\vec{R}\rangle = |\vec{R}\rangle \) for \( \delta < 0 \). The corresponding (smooth) Bloch eigenfunction \( |\psi^0_k\rangle \) are given

\[
|\psi^0_k\rangle = \langle \vec{R}|\vec{w}_0\vec{R}\rangle |\vec{w}_0\vec{R}\rangle,
\]

for \( |\psi^t_k\rangle \) (not necessarily smooth) Bloch eigenfunction. A smooth gauge \( |\psi^t_k\rangle \) for a finite value of the parameter \( t \) is obtained by parallel transport of \( |\psi^0_k\rangle \) as the hoppings are switched on

\[
|\psi^t_k\rangle = \langle \vec{R}| \prod_{\ell=0}^{t} |\vec{w}_\ell\vec{R}\rangle \langle \vec{w}_\ell\vec{R}| |\psi^0_k\rangle \langle \psi^0_k| |\psi^t_k\rangle.
\]

We set \( t = -0.08 \) and drop the superscript \( t \) from now on. The bulk WF takes the form

\[
|\vec{w}_{\vec{R}}\rangle = \sum_{\vec{k}} e^{i\vec{k}\cdot\vec{R}} |\vec{k}\rangle.
\]
Inspecting the values of $|\tilde{w}_{(0,0)}(\vec{R})|^2$ for different unit-cells, we observe that the obtained WF is well localized, with 99.5% of the charge lying within the unit-cell at (0, 0). Using Eq. (14), we obtain the bulk quadrupole tensor $\hat{q}$ with components in ($\vec{a}_1, \vec{a}_2$)-basis

$$\hat{q}_{12} = \hat{q}_{21} = -1.65919 \times 10^{-3} e, \tag{37}$$

$$\hat{q}_{11} = \hat{q}_{22} = -7.34447 \times 10^{-3} e, \tag{38}$$

where we assumed the ion charge $e$ is localized at $\vec{R}$.

**Edges along primitive vectors $\vec{a}_1$ and $\vec{a}_2$.**—We now perform ribbon calculation, for a ribbon with periodic boundary conditions along $\vec{a}_1$-direction, and the supercell consisting of unit-cells at positions $R_2 \in [-N_2, N_2]$, $N_2 = 20$. The Fourier transform of Eq. (33) gives Bloch Hamiltonian $\hat{h}_{k\alpha}$. Substituting the bulk WF $|\tilde{w}_{k\alpha}(\vec{R})|$ into Eq. (25), the hybrid bulk WF $|\tilde{w}_{k\alpha}(\vec{R})|$ is obtained. We find that the projector (26) $\tilde{P}_{k\alpha}^{L}$ for $L = 14$ satisfies the criteria (27) and (29) both with accuracy of $10^{-12}$. From Eq. (28), the edge projector onto the top edge along $\vec{a}_1$, $\tilde{P}_{k\alpha}^{\text{edge}}$, is obtained, giving the Wannier edge polarization

$$\tilde{P}_{\alpha}^{\text{edge}} = (0.17609\vec{a}_1 + 3.24851\vec{a}_2) \times 10^{-3} e, \tag{39}$$

where in Eq. (6) we used the grid of 120 equally spaced $k_1$-points. (In this section we index the (Wannier) edge polarizations with the corresponding edge lattice vector instead of the integer index.) The same procedure is repeated for the right edge along $\vec{a}_2$, which gives $\tilde{P}_{\alpha}^{\text{edge}}$ obtained from Eq. (39) after setting $\vec{a}_\alpha \rightarrow \vec{a}_\alpha$. Substituting Eqs. (37)-(39) into the expression for the edge polarization (3), gives

$$\tilde{F}_{\alpha}^{\text{edge}} = (-0.65350\vec{a}_\alpha - 0.42372\vec{a}_\alpha) \times 10^{-3} e. \tag{40}$$

**Edge along $\vec{e}_1 = 2\vec{a}_1 + \vec{a}_2$**—We consider a ribbon, periodic in $\vec{e}_1 = 2\vec{a}_1 + \vec{a}_2$ direction, with supercell along $\vec{a}_1$-direction. Repeating the same calculation as above, we obtain for $N_2 = 30$, that choosing $L = 15$ satisfies conditions (27) and (29) both with accuracy of about $10^{-8}$. The Wannier edge polarization for the upper edge of this ribbon is

$$\tilde{P}_{\alpha}^{\text{edge}} = (6.05756\vec{e}_1 - 14.76152\vec{a}_1) \times 10^{-3} e. \tag{41}$$

The above result together with Eqs. (3) and (37)-(38), give the edge polarization $\tilde{F}_{\alpha}^{\text{edge}}$ for the edge along $\vec{e}_1$

$$\tilde{F}_{\alpha}^{\text{edge}} = (-0.45731\vec{e}_1 + 0.28122\vec{a}_1) \times 10^{-3} e. \tag{42}$$

**Edge along $\vec{e}_1 = 2\vec{a}_1 - \vec{a}_2$**—Proceeding as above, we obtain for the Wannier edge polarization for the upper edge of the ribbon along $\vec{e}_1$

$$\tilde{P}_{\alpha}^{\text{edge}} = (-6.76134\vec{e}_1 + 17.14810\vec{a}_1) \times 10^{-3} e, \tag{43}$$

and the corresponding edge polarization,

$$\tilde{F}_{\alpha}^{\text{edge}} = (1.41273\vec{e}_1 - 4.52168\vec{a}_1) \times 10^{-3} e. \tag{44}$$

**Edge dipole $D_{\text{edge}}$**—We confirm that the relation (5) holds exactly. For example, for the edges along the lattice vectors $\vec{a}_\alpha$

$$\frac{L_\alpha}{A_{\text{cell}}} \tilde{P}_{\alpha}^{\text{edge}} \cdot \vec{n}_\alpha = -0.42372 \times 10^{-3} e, \tag{45}$$

agrees with the value obtained from either flake or ribbon calculation $L_1 L_2^D_{\alpha} = L_0 L_2^D_{\alpha} = -0.42372 \times 10^{-3} e$.

**Corner charge.**—Three different corners, as shown in Fig. 6, are considered. We denote the edge lattice vectors by $\vec{e}_\alpha$ for the two edges, $\alpha = 1, 2$, meeting at the corner, and $A_{\text{cell}} = |\vec{e}_1 \times \vec{e}_2|$ is the area of the unit-cell defined by the corner. To compute the corner charge, we consider a flake with the boundaries along the edge vectors, with the lower-left corner located at $-N_1\vec{e}_1 - N_2\vec{e}_2$ and the upper-right corner at $N_1\vec{e}_1 + N_2\vec{e}_2$. After diagonalization of the Hamiltonian (33) for $N_1 = N_2 = 20$, the charge density $\rho(\vec{x})$ is obtained using eigenvectors with the components $\psi_n(\vec{x})$,

$$\rho(\vec{x}) = -e \sum_{\vec{R}, n=1}^{N_{\text{occ}}} (|\psi_n(\vec{R})|^2 - 1) \delta(\vec{x} - \vec{R}), \tag{46}$$

where $N_{\text{occ}} = (2N_1 + 1)(2N_2 + 1)$, and the term $"-1$" is the contribution from the ions assumed to be localized at the positions $\vec{R}$.
For the situation in Fig. 6a, the corner charge $Q_c^c$ is obtained by integrating the charge density (46) over the corner area denoted by dashed lines. Since both orbitals have the same position within the unit-cell, there is no contribution from the ramp functions, see Sec. II B. We obtain $Q_c^c = -1.30687 \times 10^{-3} e$ which should be compared with Eq. (4),

$$Q_c^c = \frac{L_2}{A_{cell}} \rho_{\text{edge}} \cdot \vec{n}_2 + \frac{L_1}{A_{cell}} \rho_{\text{edge}} \cdot \vec{n}_1 = -1.30700 \times 10^{-3} e,$$

(47)

where $L_\alpha = |\vec{a}_\alpha|$, and $\vec{n}_\alpha$ is unit normal vector as depicted in Fig. 6a.

Figure 6b-c considers the corner formed by the edges $\vec{c}_1 = 2\vec{a}_1 + \vec{a}_2$ and $\vec{c}_2 = \vec{a}_2$. For the corner region as in Fig. 6b, we pass the charge density (46) through Gaussian filter and integrate over the corner region, which yields the same result as simply integrating the microscopic charge density (46) over the corner region. The resulting corner charge $Q_c^c = -1.11059 \times 10^{-3} e$ should be compared with

$$Q_c^c = \frac{L_1}{A_{cell}} \rho_{\text{edge}} \cdot \vec{n}_1 + \frac{L_1}{A_{cell}} \rho_{\text{edge}} \cdot \vec{n}_1 = -1.11081 \times 10^{-3} e. $$

(48)

On the other hand, for the corner region in Fig. 6c, the corner charge $Q_c^c$ can be either obtained by multiplying the charge density (46) by the product of ramp functions, see Sec. II B, or by passing it through Gaussian filter and then integrating. The result $Q_c^c = -0.75898 \times 10^{-3} e$ agrees well with

$$Q_c^c = \frac{L_2}{A_{cell}} \rho_{\text{edge}} \cdot \vec{n}_2 + \frac{L_2}{A_{cell}} \rho_{\text{edge}} \cdot \vec{n}_2 = -0.75834 \times 10^{-3} e, $$

(49)

where $L = |\vec{c}_1|$, and $\vec{n}$ is the unit normal vector as shown in Fig. 6c.

The third corner that we consider is shown in Fig. 6d-e, formed by the lattice vectors $\vec{c}_1^d = 2\vec{a}_1 - \vec{a}_2$ and $\vec{c}_2^d$. For the corner region defined by the line along $\vec{a}_1$, see Fig. 6d, the corner charge is obtained by integrating the microscopic charge density over the corner region, which gives $Q_c^d = -0.75806 \times 10^{-3} e$. On the other hand, from bulk-and-edge to corner charge correspondence (4), we obtain

$$Q_c^d = \frac{L_1}{A_{cell}} \rho_{\text{edge}} \cdot \vec{n}_1 + \frac{L_1}{A_{cell}} \rho_{\text{edge}} \cdot \vec{n}_1 = -0.75923 \times 10^{-3} e, $$

(50)

where we used that the edge polarization for the left edge along $\vec{a}_2$ in Fig. 6a is minus that of the right edge, i.e., $-\rho_{\text{edge}}$. This relation holds for the present example because the system is inversion symmetric. Finally, for the corner region in Fig. 6e, we perform moving window average of the microscopic charge density and integrate it over the corner region. The resulting corner charge $Q_c^e = 1.71431 \times 10^{-3} e$ agrees with

$$Q_c^e = \frac{L_1}{A_{cell}} \rho_{\text{edge}} \cdot \vec{n}_1 + \frac{L_2}{A_{cell}} \rho_{\text{edge}} \cdot \vec{n}_1 = 1.71347 \times 10^{-3} e. $$

(51)

In the above expression we used the notation $L' = |\vec{c}_1^e|$, and the unit-normal vector $\vec{n}^e$ is shown in Fig. 6e.

Flake’s quadrupole moment tensor—For comparison, we also compute the quadrupole tensor for the inversion symmetric flake shown in Fig. 6a

$$q_{12}^{\text{flake}} = q_{12}^{\text{flake}} = -1.1582 \times 10^{-3} e, $$

(52)

$$q_{11}^{\text{flake}} = q_{22}^{\text{flake}} = -7.43307 \times 10^{-4} e. $$

(53)

We observe that neither $q_{12}^{\text{flake}}$ agrees well with the corner charge $Q_c^a$, nor $q_{11}^{\text{flake}}/2$ with the edge dipole $L_1 L_1^{\text{edge}}$ for the flake size $N_1 = N_2 = 20$, see Sec. III C.

B. Orbitals with internal quadrupole moment

In the previous example we assumed that the orbitals of the tight-binding model (33) are isotropic, hence they themselves have vanishing quadrupole moment with respect to their center-of-mass. To include possible quadrupole moments of the electron orbitals, we can replace the corresponding delta function for the electrons in Eq. (46) with the actual shape of the orbitals’ charge density. Alternatively, we can perform following unitary transformation to Hamiltonian (33) which changes the basis from $|\vec{R}\alpha\rangle$ to $|\vec{R}\tilde{\alpha}\rangle$,

$$|\vec{R}\rangle = \frac{1}{\sqrt{2}}(|\vec{R}\tilde{1}\rangle + |\vec{R}\tilde{2}\rangle), $$

(54)

$$|\vec{R}\rangle = \frac{1}{\sqrt{2}}(|\vec{R}\tilde{1}\rangle - |\vec{R}\tilde{2}\rangle). $$

(55)

Since inversion symmetry maps the two new orbitals as $\tilde{1} \leftrightarrow \tilde{2}$, one can move the orbitals $|\vec{R}\tilde{\alpha}\rangle$ to the positions $\vec{R} + (-1)^\alpha \vec{X}$, where $\vec{X} = X_1 \hat{a}_1 + X_2 \hat{a}_2$ with $X_1, X_2 \in [-1/2, 1/2]$. The obtained tight-binding model is the same as the model (33), although it has quadrupole moment tensor with components in reduced coordinates equal to $q_{12} = q_{21} = -eX_1 X_2$, $q_{11} = -eX_1^2$ and $q_{22} = -eX_2^2$ for the case when all the hoppings are set to zero.

In order to calculate the corner charge $Q_c$ of a flake for the top-right corner in Fig. 6a, we proceed as in the previous section, where now instead of the charge density (46) we have

$$\rho(\vec{x}) = -e \sum_{\vec{R}, \alpha} \langle |\vec{R}\tilde{\alpha}\rangle |\psi_{\alpha}\rangle^2 \delta(\vec{x} - \vec{R} - (-1)^\alpha \vec{X}) $$

(56)

After multiplying the above charge density with the product of ramp functions $f_1(x_1) f_2(x_2)$ and integrating over the whole space, see Sec. II B, we obtain the corner charge of the flake

$$Q_c = Q_c^a + 0.0101783 e \times (X_1 + X_2) - eX_1 X_2, $$

(57)

where $Q_c^a$ is the corner charge (47) for the case when both the orbitals are placed at position $\vec{R}$, i.e. $\vec{X} = 0$. Similarly, the
calculation of the bulk quadrupole tensor, using the WF from the previous example, gives
\[
\hat{q}_{12} = 
\hat{q}_{21} = \hat{q}_{12}^{(0,0)} - eX_1X_2, \quad (58) \\
\hat{q}_{11} = \hat{q}_{11}^{(0,0)} - eX_1^2, \quad (59) \\
\hat{q}_{22} = \hat{q}_{22}^{(0,0)} - eX_2^2, \quad (60)
\]
where the superscript "(0,0)" denotes the quadrupole moment tensor in Eqs. (37)-(38). The calculation of Wannier edge polarization has additional contribution from the second term in Eq. (6)
\[
\hat{P}^{\text{edge}}_{\vec{a}_\alpha} = \hat{P}^{\text{edge},(0,0)}_{\vec{a}_\alpha} + 0.0101784e \times \vec{X}, \quad (61)
\]
where the term \(\hat{P}^{\text{edge},(0,0)}_{\vec{a}_\alpha}\) is given by Eq. (39). Similarly, the edge polarization \(\hat{P}^{\text{edge},(0,0)}_{\vec{a}_\alpha}\) gets modified to
\[
\hat{P}^{\text{edge}}_{\vec{a}_\alpha} = \hat{P}^{\text{edge},(0,0)}_{\vec{a}_\alpha} + 0.0101784e \times \vec{X} - \frac{1}{2} eX_2^2 \vec{a}_\alpha \\
- \frac{1}{2} eX_1X_2 \vec{a}_\alpha, \quad (62)
\]
The bulk-and-edge to corner charge correspondence (4) gives the corner charge
\[
Q_c = \frac{L_2}{A_{\text{cell}}} \hat{P}^{\text{edge}}_{\vec{a}_1} \cdot \vec{n}_2 + \frac{L_1}{A_{\text{cell}}} \hat{P}^{\text{edge}}_{\vec{a}_2} \cdot \vec{n}_1 \quad (63)
\]
\[
= Q^a_{\alpha} + 0.0101784e \times (X_1 + X_2) - eX_1X_2, \quad (64)
\]
which agrees well with the independent corner charge calculation (57).

Note that the model studied in this example for \(X_1 = X_2 = 1/6\), is the same as the model previously studied in Ref. 26, although here we chose different hopping parameters. We are now in position to understand why the contribution from the bulk quadrupole tensor \(\hat{q}\) was previously overlooked. Reference 26 assumes that \(e/2\) ionic charge is localized at each lattice site instead of ionic charge \(e\) localized at \(\vec{R}\) as it was done in Eq. (56). Therefore, the charge density (56) is modified to
\[
\rho(\vec{x}) = -e \sum_{\vec{R},\vec{n}} \left( |\langle \vec{R}\alpha | \psi_n \rangle|^2 - \frac{1}{2} \right) \delta(\vec{x} - \vec{R} - (-1)^\alpha \vec{X}). \quad (65)
\]
The resulting corner charge \(Q_c\) is given by Eq. (57) with the last term \(-eX_1Y_1\) omitted. The above modification of the ionic charge density changes the expressions for the quadrupole tensor \(\hat{q}\) in Eqs. (58)-(60) to \(\hat{q}^{(0,0)}\). Therefore, Eq. (62) becomes
\[
\hat{P}^{\text{edge}}_{\vec{a}_\alpha} = \hat{P}^{\text{edge},(0,0)}_{\vec{a}_\alpha} + 0.0101784e \times \vec{X}, \quad (65)
\]
where the dominant contribution is from the \(\vec{X}\)-dependent piece of the corresponding Wannier edge polarization (61). Although for the hopping parameters chosen in this example, the bulk contribution \(\hat{q}^{(0,0)}\) from \(\hat{P}^{\text{edge},(0,0)}\) cannot be overlooked for \(X_1 = X_2 = 1/6\), that is not the case for the hopping parameters used in Ref. 26. This statement should be compared to Eq. (63), where \(\vec{X}\)-dependent bulk contribution \(-eX_1X_2\), dominates.

V. CONCLUSIONS

The statement of bulk-boundary correspondence, formulated by modern theory of electrical polarization, is that the non-vanishing bulk polarization of a two-dimensional insulator determines the edge charge density. On the other hand, for vanishing bulk polarization one can observe bound-ary signatures in form of corner charges and edge dipoles. In this work we prove that corner charges and edge dipoles of band insulators can be obtained by representing the terminated crystal as collection of edge regions with polarization \(\hat{P}^{\text{edge}}_{\alpha}\), where \(\alpha\) enumerates the edges (see Fig. 1). We find that the edge polarization \(\hat{P}^{\text{edge}}_{\alpha}\) consists of two pieces, the bulk piece given by the quadrupole tensor of bulk Wannier functions’ charge density, and the edge piece that we call Wannier edge polarization \(\hat{P}^{\text{edge}}_{\alpha}\). The Wannier edge polarization is defined as polarization of the edge subsystem, which is obtained by cutting out the region around the corresponding edge using “Wannier cut”, the cut that utilizes the bulk Wannier functions as “shape cutter”. Within our representation of the terminated crystal, the edge polarizations \(\hat{P}^{\text{edge}}_{\alpha}\) determine the corner charges via mentioned bulk-boundary correspondence. Since \(\hat{P}^{\text{edge}}_{\alpha}\) has both bulk and edge piece, the resulting correspondence (4) is dubbed bulk-and-edge to corner correspondence, which is the main result of our work. The edge polarizations \(\hat{P}^{\text{edge}}_{\alpha}\) defined in this work, depend on the choice of occupied bulk Wannier functions which is consistent with the fact that the number of physical observables (i.e. corner charges and edge dipoles) is one less than the number of independent components of all the edge polarizations.

In the context of this work, only the corner charges and the edge dipole moments are considered as relevant physical observables characterizing the macroscopic charge density of a terminated crystal. For this reason, only the lowest non-vanishing multipole moment, polarization in this case, is taken into account for the edge regions in Fig. 1. For example, one can represent the crystal as collection of edge regions that have not only polarization but also quadrupole moment. Although the quadrupole moment of the edge region affects neither the corner charge nor the edge dipole, see Fig. 4, it does affect finer (higher-order) features of the flake’s macroscopic charge density. Admittedly, even the measurement of corner charges and edge dipoles may prove to be experimentally challenging. Here we imagine a setup consisting of a crystal with \(n\) edges, where application of strain causes the edge polarizations (3) to change. The change in the edge polarizations results in the current-flow along the corresponding edge, which can be in principle measured. The measurement of the currents related to the change of the edge dipole requires more local current probes which poses an additional difficulty.

In this work, we considered two-dimensional systems and we expect the extension to three-dimensional systems to follow along the similar lines. Namely, for three-dimensional crystal with vanishing bulk polarization, one can consider hinge charge density, or in the case the hinge charge density vanishes, the corner charges. In the former case, the aim
would be to represent the terminated crystal as collection of polarized surface regions, whereas in the latter case one would have polarized hinge regions. Another interesting question in this context is finding all the symmetry constraints that quantize some of the mentioned boundary signatures, where the bulk Wannier functions can be chosen to respect the symmetry constraint. On a more challenging side, we mention the bulk Wannier functions can be chosen to respect the symmetry constraints that quantize some of the mentioned boundary signatures, where the this context is finding all the symmetry constraints that quantize some of the mentioned boundary signatures, where the

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