Visualizing intrinsic Hall currents in simple lattices

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The topological properties of a material’s electronic structure are encoded in its Berry curvature, a quantity which is intimately related to the transverse electrical conductivity. In this paper we identify a previously unrecognized consequence of Berry curvature: an electric field-induced change in the electrons’ charge density orientation. This charge density response applies to lattices composed of monoatomic unit cells with orbitals of the same character (e.g., p-like or d-like). Based on this picture, the formation of the intrinsic anomalous Hall current in ferromagnets can be understood in terms of the real space re-orientation of the charge density. We also show that measurements of the electric field-induced change in charge density of monolayer transition metal dichalcogenides can be used to measure the Berry curvature and valley Hall conductivity of these materials.

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Introduction – The topological description of electronic structure provides a powerful framework with which to understand basic material properties. A foundational example is the anomalous Hall effect, in which an applied electric field \( \mathbf{E} \) in a ferromagnet with magnetization \( \mathbf{M} \) results in electrical current flowing along the \( \mathbf{E} \times \mathbf{M} \) direction. Despite the anomalous Hall effect being observed over a century ago, its topological origins were only understood in recent decades [1]. In this example and others, a material’s topological properties are inferred from transport measurements. This is a natural consequence of the fact that the mathematical quantity that encodes the topological character of a state - the Berry curvature - can be written in terms of the transverse electrical conductance. There are, however, numerous systems with nontrivial Berry curvature which exhibit no net electrical response [2]. Prominent examples are found in certain structural phases of 2-dimensional transition metal dichalcogenides with broken inversion symmetry, which possess nonzero Berry curvature, but whose time reversal symmetry ensures no net electrical response [3]. In this case, the electronic structure topology leads to another type of Hall effect - the valley Hall effect - in which states with opposite orbital angular momentum flow in opposite directions along the \( \mathbf{E} \times \mathbf{z} \) axis [4, 5], where \( \mathbf{z} \) is perpendicular to the layer. This and similar flavors of Hall effect (e.g., spin Hall effect [6, 7]) are typically more subtle to observe, relying on methods including optical detection of orbital or spin angular momentum accumulation at sample boundaries [8, 9].

In this paper we identify a previously unrecognized consequence of Berry curvature: an electric field-induced change in the electrons’ charge density orientation. The response we derive applies to lattices composed of a monoatomic unit cell with orbitals of the same character (e.g., p-like or d-like); we refer to such lattices as “simple lattices”. Although these are restrictive assumptions, they pertain to cases of practical interest, such as near-band edge states in transition metal dichalcogenides, or \( d \)-bands in transition metal ferromagnets [10]. For simple lattices, we derive a general relationship between the real space density \( \rho(\mathbf{r}) \) of a wave function and its velocity \( \mathbf{v} \), which in turn is directly related to the Berry curvature. Thus, the relationship we derive relates the Berry curvature to the electric field-induced change in real space density, providing a new route to probing the topological properties of materials. As an application, we first analyze ferromagnetic systems and relate the real space density response of individual states to their anomalous Hall response. We then consider transition metal dichalcogenide monolayer and demonstrate that the electric field-induced change in charge density can be utilized as a quantitative measure of this material’s Berry curvature, or equivalently the valley Hall conductivity.

Formalism – In this section we present the precise connection between the Berry curvature and the electric field-induced change in real space density. We begin with the relation between a state’s real space density \( \rho(\mathbf{r}) \) and its velocity. There is generally no reason to expect any relation between these quantities; a general wave function \( \psi(\mathbf{r}) = A(\mathbf{r}) \exp(i\phi(\mathbf{r})) \) (with \( A, \phi \) real) possesses a charge density \( A(\mathbf{r})^2 \) and velocity \( A(\mathbf{r})^2 \nabla \phi(\mathbf{r}) \), two independent quantities. However, for an electron in a simple lattice with a given value of Bloch wave vector \( \mathbf{k} \), we show next that a state’s charge density distribution is related to its velocity.

We start with the crystal field Hamiltonian of a simple lattice. We take the basis to be real localized orbitals, such as Wannier functions or atomic orbitals, which are a product of a radial function and angular function:

\[ \phi_M(\mathbf{r}) = R_{n,\ell}(\mathbf{r}) Y^M_{\ell}(\theta, \phi), \quad (1) \]

where \( R_{n,\ell}(\mathbf{r}) \) is a radial function for states in the \( n \)th
shell with angular momentum \( \ell \). \( \gamma^M_\ell \) is the real-valued spherical harmonic, with \( 2\ell + 1 \) distinct \( M \) labels (e.g., for \( \ell = 1 \), \( M = \{ x, y, z \} \)). Note that \( M \) is sufficient to label the basis states since we assume all orbitals have the same value for \( n \) and \( \ell \). In this basis, the tight-binding crystal field Hamiltonian is:

\[
H_0(k) = \sum_{R,M,M'} \cos(k \cdot R) \ t^\sigma_{M,M'}(R) \left( c^\dagger_M c_{M'} + h.c. \right),
\]

where the sum \( R \) includes the primary unit cell (\( R = 0 \)) and all other Bravais lattice vectors. Typically the sum is truncated according to distance (e.g., up to first, second, or third nearest-neighbor). \( c^\dagger_M (\epsilon_{M'}) \) is the electron creation (annihilation) operator for orbital \( M(M') \) located in the primary unit cell. \( t^\sigma_{M,M'}(R) \) is the \( \sigma \)-hopping parameter between orbital \( M \) of the primary unit cell and orbital \( M' \) centered at lattice site \( R \). Eq. (6) includes only \( \sigma \)-hopping, however generally \( \pi \) and \( \delta \) hopping amplitudes are smaller, so that the above model is typically adequate (see Supp. Info for a comprehensive assessment of the model’s validity).

The current operator \( \mathbf{v} = d\mathbf{H}/dk \) derived from this Hamiltonian is:

\[
\mathbf{v}(k) = -\sum_{R,M,M'} R \sin(k \cdot R) \ t^\sigma_{M,M'}(R) \left( c^\dagger_M c_{M'} + h.c. \right).
\]

Each term in the sum over \( R \) represents the current flowing between the atom at \( R = 0 \) and the atom at \( R \). Note that a current between sites separated by \( R \) requires nonzero overlap between \( \mathbf{k} \) and \( \mathbf{R} \), and overlap between orbitals on the two sites. The orbital overlap is closely related to the shape of the wave function density \( \rho_0(\mathbf{r}) \):

\[
\rho_0(\mathbf{r}) = \sum_{M,M'} \left( c^\dagger_M c_{M'} + h.c. \right) \phi_M(\mathbf{r}) \phi_{M'}(\mathbf{r})
\]

where the atom center is at \( r = 0 \), and \( \rho_0^\text{rad}(r) \) is normalized such that \( \int_0^\infty r^2 \rho_0^\text{rad}(r) dr = 1 \) (so that \( \rho_0^\text{ang}(\mathbf{r}) \) is dimensionless).

In the Supp. Info., we show that the angular part of the density \( \rho_0^\text{ang}(\mathbf{r}) \) is related to the hopping parameters and wave function coefficients of Eq. (23) (the last two factors in that equation). This leads to the following relation between a state’s velocity and density:

\[
\mathbf{v}(k) = \sum_R R \sin(k \cdot R) \hat{t}^\sigma(R) \rho_0^\text{ang}(\mathbf{k},\mathbf{R}).
\]

where \( \hat{t}^\sigma(R) = t^\sigma(R)/Y_{m=0}(0,0) \) is the \( \sigma \)-hopping parameter normalized by a (known) constant factor. (Note that we added a \( \mathbf{k} \) label for \( \rho \).). \( t^\sigma(R) \) is the \( \sigma \)-dependent \( \sigma \)-hopping function whose form is semi-universal and taken as known \textit{a priori} \[14\]. In the sum over neighboring atom positions \( R \), a positive current corresponds to a state propagating outward from \( R = 0 \) to \( R = \mathbf{R} \), while a negative current corresponds to a state propagating inward from \( R = \mathbf{R} \) to \( R = 0 \).

Equation (6) is one of our primary results, and provides an intuitive relationship between a state’s charge density and current: the velocity along \( \mathbf{R} \) is the product of the wave function phase change along \( \mathbf{R} \) (given by the factor \( \sin(k \cdot R) \)) and the density along \( \mathbf{R} \) (given by the factor \( \rho_0^\text{ang}(\mathbf{k},\mathbf{R}) \)). This representation of velocity is a substantial simplification of the general form given in Eq. (23) which requires knowledge of the full hopping elements (encoded in Slater-Koster tight binding tables) and the complex wave function coefficients.

Armed with this density-velocity connection, we next turn to the relation between the Berry curvature, the intrinsic anomalous Hall effect, and a state’s velocity. The \( z \)-component of the Berry curvature \( \Omega_z^n \) of an eigenstate \( \psi_n \) is:

\[
\Omega^n_z(k) = 2 \Im \sum_{m \neq n} \langle \psi^0_n | v_x | \psi^0_m \rangle \langle \psi^0_m | v_y | \psi^0_n \rangle / (\epsilon_m - \epsilon_n)^2,
\]

where \( \epsilon_n \) is the energy of the \( n \)-th state and \( v_{x,y} = dH/dk_{x,y} \). In the clean limit, the intrinsic anomalous Hall effect is given by the sum of the occupied states’ Berry curvature: \( \sigma_{\text{AHE}} = e^2/h \sum_n f_n \Omega_{z}^n \), where \( f_n \) is the occupancy of the \( n \)-th state. The Berry curvature and anomalous Hall conductivity can also be understood in terms of perturbation theory. An applied electric field perturbs the eigenstates and may change their velocity. The linear-in-\( E \) change in velocity \( \delta \mathbf{v} \) is equivalent to the Berry curvature:

\[
\Omega^n_z(k) = (\mathbf{E}/E) \times (\delta v_z^n(k)),
\]

where \( E \) is the electric field strength.

We next invoke Eq. (6) to relate the change in velocity to a change in the charge density. Immediately we conclude that, in simple lattices, the real space density response of the \( n \)-th state is related to its Berry curvature:

\[
\Omega^n_z(k) = (\mathbf{E}/E) \times \sum_R R \sin(k \cdot R) \hat{t}^\sigma(R) \langle \delta \rho_0^\text{ang}(\mathbf{k},\mathbf{R}) \rangle.
\]

Equation (9) is another primary result, which provides the connection between a state’s Berry curvature and the electric field-induced change in its density distribution.
It’s straightforward to prove that either the change in velocity or the change in density is observable - but not both. The net change of any observable is obtained by summing over \( \mathbf{k} \). The net change in velocity yields the anomalous Hall conductivity, and is derived entirely from the component of \( \delta v(\mathbf{k}) \) that is even-in-\( \mathbf{k} \) (the odd-in-\( \mathbf{k} \) component vanishes after summation). The \( \sin(\mathbf{k} \cdot \mathbf{R}) \) factor on the right hand side of Eq. (6) indicates that \( v(\mathbf{k}) \) and \( \delta \rho_0(\mathbf{k}, \mathbf{R}) \) have opposite parity under \( \mathbf{k} \rightarrow -\mathbf{k} \). Therefore the net change in states leading to the anomalous Hall current leads to zero net change in charge density.

The converse scenario also holds: the net change in density is derived from the even-in-\( \mathbf{k} \) \( \delta \rho(\mathbf{k}, \mathbf{r}) \), which corresponds to the odd-in-\( \mathbf{k} \) \( \delta v(\mathbf{k}) \). Therefore a net change in density is associated with vanishing intrinsic anomalous Hall current. For this reason, \( \delta \rho \) becomes the observable connected to the Berry curvature for systems in which the charge current response vanishes. Recognizing \( \delta \rho \) as a signature of Berry curvature therefore expands the range of systems for which \( \Omega \) may be accessed experimentally. In the following sections we provide examples to illustrate the connection between \( \delta \rho \) and the Hall conductivity, or Berry curvature.

2-band model of a ferromagnet – We start with a toy model to illustrate Eq. (6) in practice. The model is depicted in Fig. 1(a) and consists of \( p_x \) and \( p_y \) orbitals on a square lattice. \( \sigma \)-hopping up to second nearest neighbor leads to hopping \( t \) between pairs of \( p_x \) (\( p_y \)) orbitals displaced along the \( x \)-direction (\( y \)-direction), and second nearest neighbor hopping \( t' \) between \( p_x \) and \( p_y \) orbitals (for \( \sigma \)-hopping \( t' = t/4 \)). In the small \( k \) limit, the crystal field Hamiltonian in the \( (p_x, p_y) \) basis is:

\[
H_0 = 2t'k^2\sigma_0 + \begin{pmatrix} tk_x^2 & 4t'k_xk_y \\ 4t'k_xk_y & tk_y^2 \end{pmatrix}
\]

where \( \sigma_0 \) is the identity matrix.

We assume the system is magnetized in the \( z \)-direction with an exchange splitting that is larger than all other energy scales, and consider only one spin component, \( s_z = +1 \). The spin-orbit coupling term \( s \cdot \mathbf{L} \) therefore takes the form \( \alpha L_z \), where \( \alpha \) parameterizes the spin-orbit strength.

We present an analysis of a simple case which captures the general behavior of the model (see Supp. Info for more general analysis), and which demonstrates the usage of Eq. (6). We take \( k_x = 0, k_y \neq 0 \) and suppose that the spin-orbit coupling \( \alpha \) is much less than the crystal field splitting \( tk^2 \). In this case the unperturbed eigenstates are:

\[
|\psi_1\rangle = \begin{pmatrix} -i\alpha' \\ 1 \end{pmatrix}; \quad |\psi_2\rangle = \begin{pmatrix} 1 \\ i\alpha' \end{pmatrix}
\]

where \( \alpha' = \alpha/\hbar^2 \). \( \psi_1(2) \) is composed mostly of a \( p_y \) \((p_x)\) orbital, with small orbital mixing due to spin-orbit coupling. The density of \( |\psi_1\rangle \) is shown in Fig. 1(a), and its velocity is along the \( \mathbf{k} = k\hat{y} \) direction.

An applied field in the \( y \)-direction introduces a perturbation \( qE_y \) which mixes the eigenstates and leads to a re-orientation of the charge density of each state. The change in charge density of \( |\psi_1\rangle \) is shown in Fig. 1(d). Given the perturbed density and the Bloch wave function \( \Psi(\mathbf{k}, \mathbf{r}) \), we have the ingredients needed to apply Eq. (6). The velocity from the primary unit cell atom (labelled ‘5’) to atoms ‘7’ and ‘9’ include a positive factor from \( \sin(\mathbf{k} \cdot \mathbf{R}) \). The change in density between atoms ‘5’ and ‘9’ is negative, corresponding to flow towards atom ‘5’, while the change in density between atoms ‘5’ and ‘7’ is positive, corresponding to flow away from atom ‘5’. Finally, the change in density between atoms ‘5’ and ‘8’, and atoms ‘5’ and ‘6’ is zero, so there is no change in current along those directions. The resulting bond current directions shown in the figure result in a transverse current flow in the \( x \)-direction. We can therefore understand the intrinsic anomalous Hall response of a given state in terms of the electric field-induced change in the charge density distribution.

Imaging the Valley Hall effect in TMD – We next show that in a transition metal dichalcogenide monolayer, the electric field-induced change in charge density distribution can be used to quantitatively measure the valley Hall conductivity. The monolayer transition metal dichalcogenide MoS$_2$ in the 2H phase is a nonmagnetic semiconductor. Its crystal and electronic structure are shown Fig. 2(a) and (b), respectively. The material has a direct band gap is \( \Delta = 1.7 \) eV (computed value) located at \( \mathbf{k} = \pm \mathbf{K} = \pm 4\pi/3a_0 \langle 1,0 \rangle \), where \( a_0 \) is the in-plane lat-
The following perturbed wave function for the conduction lattice constant. (Note that \(-\mathbf{K}\) is often labelled \(\mathbf{K}'\)). This material is not a simple lattice: the unit cell contains 2 Se atoms and 1 Mo atom, and there is significant \(p-d\) orbital hybridization in some regions of the band structure. However, the states near the band gap at \(\mathbf{K}\) and \(-\mathbf{K}\) exhibit the largest contribution to the Berry curvature. These states are composed primarily of \(d\)-orbitals localized on the Mo atoms, which form a simple hexagonal lattice, and which \(d\) approximately satisfy the assumptions of our analysis. The conduction band is composed of \(L_z = 0\) states, corresponding to \(|d_{z^2}\rangle\), while the valence band is \(L_z = \pm 2\) states at \(\mathbf{k} = \pm \mathbf{K}\), corresponding to \((|d_{xy}| \pm i|d_{x^2-y^2}|)/\sqrt{2}\) (see Fig. 2(c)).

In the vicinity of \(\mathbf{K}\), the conduction and valence bands are described by a massive Dirac Hamiltonian [3]. Letting \(\mathbf{q} = \mathbf{k} - \mathbf{K}\), we have:

\[
H = t_{\alpha} (q_{\alpha} \tau_{\alpha} + q_{\rho} \tau_{\rho}) + \frac{\Delta}{2} \tau_z
\]

(12)

where \(\tau\) is a Pauli matrix in the space of conduction and valence band states. We first consider the currents and charge densities of the equilibrium states at \(\mathbf{q} = 0\) (or \(\mathbf{k} = \mathbf{K}\)). The eigenstates are \(\psi_c = \begin{pmatrix} 1 \\ 0 \end{pmatrix}\) and \(\psi_v = \begin{pmatrix} 0 \\ 1 \end{pmatrix}\). The \(R \sin(\mathbf{K} \cdot \mathbf{R})\) factor of Eq. 6 contributes to the bond currents as indicated by the bond-aligned arrows Fig. 3(a)-(c). The charge density of both conduction and valence band equilibrium states is isotropic in the \(x-y\) plane, so that the bond currents are weighted equally and the net current vanishes.

Applying an electric field in the \(y\)-direction results in the following perturbed wave function for the conduction band:

\[
\psi_c' = \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \frac{qEt_{\alpha} \Delta}{\Delta^2} \begin{pmatrix} 0 \\ 1 \end{pmatrix};
\]

(13)

As we will show in detail, the perturbed wave function exhibits an anisotropic \(\rho(\mathbf{r})\) which overlaps unevenly with the nearest neighbor bonds. This in turn breaks the balance of bond currents between nearest neighbors and enables a nonzero net current, corresponding to the transverse conductance or Berry curvature \(\Omega(\mathbf{K})\). The modification of the density for electric fields along \(x\) and \(y\)-directions is depicted schematically in Fig. 3(b) and (c), and provides an intuitive rationale for the formation of Hall current at the \(\mathbf{K}\) point. [5,9].

To test the quantitative validity of Eq. 6 for MoS\(_2\), we compute the electric field-induced change in charge density of the conduction band state at \(\mathbf{K}\) using the first principles tight-binding Hamiltonian and real space orbitals obtained with Quantum Espresso [12] and Wannier90 [13]. Fig. 4(a) shows isosurface contours of the electric field-induced change in density for the conduction band state at \(\mathbf{k} = \mathbf{K}\), for an applied electric field along the \(y\)-direction. Fig. 4(b) shows \(\delta \rho\) in the plane of the Mo atoms, and Fig. 4(c) shows the density \(\delta \rho(\mathbf{x})\) along a line connecting nearest neighbors. From \(\delta \rho(\mathbf{x})\) profile, we extract the (normalized) radial part \(\delta \rho^{\text{rad}}(r)\) to obtain \(\delta \rho^{\text{ang}}(\mathbf{R})\). Applying Eq. 6 leads to

\[
\Omega(\mathbf{K}) = a_0 e \frac{\delta \rho^{\text{ang}}(\mathbf{K})}{qE}
\]

(14)

We use a value of \(t^* = 0.9\) eV obtained from Wannier90. Plugging in numbers we obtain \(\Omega = 0.061\) nm\(^2\), compared to the directly computed result of \(\Omega = 0.094\) nm\(^2\). We find semi-quantitative agreement between the two values, and trace the difference back to the nonzero contribution of the \(p\) orbitals of the wave function at \(\mathbf{K}\).

The full 3-dimensional change in charge density at sub-nm length scales is not easily experimentally accessible. A relevant measurement technique for this length scale is scanning tunneling microscopy (STM). STM measures charge density of all states at a given energy (i.e., the local density of states, or LDOS), providing 2-d maps in \(xy\) position space in which the charge density along the \(z\)-direction is averaged through some convolution function.
Fig. 4(d) shows the numerical result of summing over all states at an energy 17 meV below the valence band maximum, and performing a simple integration over the $z$-direction. In the Supp. Info, we show that this data can provide an estimate of the Berry curvature, in terms of $z_{\text{max}}$, and performing a simple integration over all states at an energy 17 meV below the valence band edge. The important features are the position of $x_{\text{max}}$ and $\delta$ LDOS/qE at this position.

\[ \Omega(K) = 122.07 \times \Delta^2 q^4 \left( \frac{\delta \text{LDOS}(x_{\text{max}})}{qE} \frac{1}{D_K} \right)^2 \]

where $D_K = Am_K^*/\pi \hbar^2$ is the density of states from $\pm K$ bands; here $A$ is the unit cell area and $m_K^*$ is the effective mass at the $\pm K$ valence band. Using the numerically computed effective mass, we find an estimate of the valley hall conductivity based on the data of Fig. 4(d) to be $\Omega(K) = 0.082 \text{ nm}^2$, again comparing well to the numerically computed value of 0.094 nm$^2$.

**Conclusion** – In this work we studied the real space implications of Berry curvature for systems comprised of simple lattices. Our central finding is that the electric field-induced change in a state’s charge density distribution is directly related to its Berry curvature. This view provides a route for direct measurements of the Berry Curvature (or valley Hall conductivity) in transition metal dichalcogenide monolayers. The direct measurement of Berry curvature of these materials would assist other measurements of the valley Hall conductivity, and assist in determining other important materials properties, such as valley lifetime.

Finally, we note relevant recent work which formulates the anomalous Hall conductivity as a local property, providing a formal definition of this quantity without reference to Bloch wave vector $k$ [14][16]. This leads to a real space picture of the anomalous Hall conductivity (or “topological marker”). The formal structure of this includes the response of the second order cumulant of the charge density, resembling the picture we describe of a change in the charge density distribution. The present work straddles between the limiting cases of the more standard formulation of Berry curvature strictly in $k$-space and the work by Resta et al. [14][15], which resides entirely in real space.
Supplementary Information for "Visualizing intrinsic Hall currents in simple lattices"

RELATION BETWEEN DENSITY AND CURRENT

In this section we provide a derivation of the relation between a state’s charge density distribution and its velocity in a tight-binding model. This relation holds only for a crystal field Hamiltonian with \( \sigma \)-hopping, and is therefore qualitatively valid for cases in which \( t^\sigma, t^\delta \) are sufficiently less than \( t^\sigma \) bonding. This is often the case, and in the next section we provide an explicit description of the validity of this assumption.

The tight-binding model is represented in real-valued spherical harmonics. We denote these by \( Y_\ell^m \), which are linear combinations of \( Y_\ell^m \) and \( Y_\ell^{-m} \). Letting \( m = |M| \):

\[
Y_\ell^M = \begin{cases} 
\frac{1}{\sqrt{2}} \left( Y_\ell^{-m} + (-1)^m Y_\ell^m \right) & M < 0, \\
Y_\ell^0 & M = 0, \\
\frac{1}{\sqrt{2}} \left( Y_\ell^{-m} - (-1)^m Y_\ell^m \right) & M > 0.
\end{cases}
\]

The specific forms of the real spherical harmonics for a given \( \ell \) can be found in various references. Generally the \( M \) label is expressed in terms of the cartesian factors corresponding to the form of the spherical harmonic (e.g. for \( \ell = 1 \), \( M = \{-1,0,1\} \) is labeled as \( \{x,z,y\} \)).

In the tight-binding formulation, the \( \sigma \)-bonding hopping parameter \( t^\sigma \) is defined as the hopping between \( m = 0 \) orbitals displaced along the \( z \)-direction.

\[
t^\sigma (R) = \int dr \ V(r) \ Y_\ell^0(r) \ Y_\ell^0(r - R\hat{z}) R_{\alpha,\ell}(r) \ R_{\alpha,\ell}(r - R\hat{z})
\]

The \( t^\sigma \) hopping between orbital \( \alpha \) and \( \beta \) displaced along the \( \hat{n} \) direction is then determined by projecting each orbital along the \( |\ell, m = 0\rangle_{\hat{n}} \) (see Fig. 5(a) and (b)). This projection is obtained by rotating the \( |\ell, m = 0\rangle_{\hat{n}} \) into the \( \hat{n} \)-direction (see Fig. 5) We review this procedure next.

We denote the axis of quantization \( \hat{n} \) for the spherical harmonic in the subscript of the ket: \( |\ell, m\rangle_{\hat{n}} \). The operator which rotates \( |\ell, m\rangle_{\hat{n}} \) into \( |\ell, m\rangle_{\hat{z}} \) is denoted by \( R(\hat{n}) \):

\[
|\ell, m\rangle_{\hat{n}} = R(\hat{n}) |\ell, m\rangle_{\hat{z}}
\]

The rotated spherical harmonic \( |\ell, m\rangle_{\hat{n}} \) can be written as a linear combination of unrotated spherical harmonics with the same value of \( \ell \), written in terms of the Wigner D-matrix:

\[
R(\hat{n}) |\ell, m\rangle_{\hat{z}} = |\ell, m\rangle_{\hat{n}} = \sum_{m'} D_{m, m'}^{\ell} (\hat{n}) |\ell, m'\rangle_{\hat{z}}
\]

Crucially, for \( m = 0 \) the elements of \( D_{m=0, m'}^{\ell} \) are equal to the value of the spherical harmonic \( |\ell, m'\rangle \) evaluated at \( \hat{n} = (\theta, \phi) \).

\[
|\ell, m = 0\rangle_{\hat{n}} = \sum_{m} (Y_{\ell}^{m} (\theta, \phi))^* |\ell, m\rangle_{\hat{z}}
\]

The projection of \( |\ell, m = 0\rangle_{\hat{n}} \) onto orbital \( |\ell, m\rangle_{\hat{z}} \) is then given by Eq. 20. As described in the previous paragraph, this quantity provides the angular dependence of the hopping between orbitals displaced by \( \mathbf{R} \).

\[
\langle \ell, m | \ell, m = 0 \rangle_{\hat{n}} = (Y_{\ell}^{m})^* (\theta, \phi)
\]
FIG. 5: Depiction of the how hopping between a pair of $p_x$ orbitals is decomposed into $\sigma$ and $\pi$ contributions.

The $\sigma$-hopping contribution between orbital $\alpha$ and $\beta$ displaced by $\mathbf{R}$ is therefore equal to $y_\alpha(\hat{\mathbf{R}})$ and $y_\beta(\hat{\mathbf{R}})$:

$$t_{\sigma,M,M'}^\sigma(\mathbf{R}) = t_{\sigma}^\sigma \left( \frac{Y_M^\dagger(\hat{\mathbf{R}}) Y_{M'}(\hat{\mathbf{R}})}{Y_0^\dagger(\hat{\mathbf{R}}) Y_0(\hat{\mathbf{R}})} \right).$$  (22)

The denominator of Eq. 22 is a normalization factor that ensures that Eq. 17 is recovered for hopping between $m = 0$ orbitals displaced along the $z$-direction (i.e., for $\theta = \phi = 0$).

This form of $t$ leads to the relation between current and density. We write the general form of the current:

$$\mathbf{v}(k) = -\sum_{\mathbf{R},M,M'} \mathbf{R} \sin(k \cdot \mathbf{R}) \ t_{\sigma,M,M'}^\sigma(\mathbf{R}) \left( c_M^\dagger c_{M'} + \text{h.c.} \right)$$  (23)

Next we write the equation for the density from primary unit cell orbitals:

$$\rho_0(\mathbf{r}) = \sum_{M,M'} \left( c_M^\dagger c_{M'} + \text{h.c.} \right) Y_\ell^M(\hat{\mathbf{r}}) Y_{\ell'}^M(\hat{\mathbf{r}}) R_{n,\ell}(r) R_{n',\ell'}(r)$$

$$= R_{n,\ell}(r)^2 \sum_{M,M'} \left( c_M^\dagger c_{M'} + \text{h.c.} \right) Y_\ell^M(\hat{\mathbf{r}}) Y_{\ell'}^M(\hat{\mathbf{r}}).$$  (24)

As described in the main text, the charge density is the product of a radial function and an angular function

$$\rho_0(\mathbf{r}) = \rho_0^{\text{rad}}(r) \rho_0^{\text{ang}}(\hat{\mathbf{r}})$$

where $\rho_0^{\text{rad}}(r) = R_{n,\ell}(r)^2$ and

$$\rho_0^{\text{ang}}(\hat{\mathbf{r}}) = \sum_{M,M'} \left( c_M^\dagger c_{M'} + \text{h.c.} \right) Y_\ell^M(\hat{\mathbf{r}}) Y_{\ell'}^M(\hat{\mathbf{r}}).$$  (27)

Combining Eqs. 22, 23, and 27 we obtain:

$$\mathbf{v}(k) \propto -\sum_{\mathbf{R}} \frac{t_{\sigma}(\mathbf{R})}{Y_\ell^\dagger(0,0)^2} \mathbf{R} \sin(k \cdot \mathbf{R}) \rho_0^{\text{ang}}(\hat{\mathbf{R}})$$  (28)

$t_{\sigma}(\mathbf{R})$ is the $R$-dependent value of the sigma-bonding hopping integral, whose generally parameterized form can be found in the following section.

LIMIT OF VALIDITY FOR $\sigma$-HOPPING TIGHT-BINDING

The previous derivation applies for $\sigma$-hopping. Generally $\pi$ and $\delta$-hopping are quantitatively, and even qualitatively as important as $\sigma$-hopping. The relative importance of different hopping terms depends on the type of inter-orbital hopping and the relative orientation of the two orbitals. Fig. 6 shows both the $\sigma$-hopping and total hopping amplitudes for all of the unique interorbital hopping for $\ell = 1$, as a function of relative orientation (parameterized by polar angles $(\theta, \phi)$). The form of the tight-binding matrix elements are taken from [11]. For $p$-orbitals, the parameterization is: $V_{p\sigma} = 3.24$, $V_{pp\pi} = -0.81$, and the hopping is [11]:

$$t_{pp\sigma}(R) = V_{pp\sigma} \frac{\hbar^2}{2mR^2}$$  (29)
FIG. 6: Comparison of the total hopping (left side of each subplot) to σ-hopping (right side of each subplot) as a function of the relative orientation (parameterized by polar angles (θ, φ) for all unique pairs of p-orbitals.

Fig. 7 shows that for p-orbitals, the σ-hopping is always a good semi-quantitative estimate of the total hopping for all configurations. For ℓ = 2 (d-orbitals), the parameters are taken to be $V_{ddσ} = -16.2$, $V_{ddπ} = 8.75$, $V_{ddδ} = -2.3$, and the hopping is

$$t_{ddα}(R) = V_{ddα} \frac{h^2 R^3}{2mR^6}$$

where $R_d$ is another parameter, and is typically element-specific. A similar conclusion of the predominance of σ-hopping is reached for d orbitals, with one notable exception: the $d_{xz} - d_{x^2-y^2}$ total hopping and σ-hopping are off by a minus sign for most orbital configurations. However for all other orbital pairs, the σ-hopping at least qualitatively, and often semi-quantitatively provides a representation of the total hopping.

REAL SPACE DENSITY CALCULATIONS

We describe the procedure used to obtain the real space density associated with the perturbed eigenstates. We first obtain the real space orbitals from Wannier90, extending out 2 unit cells away from the atom center $φ_α(r)$ (so that the density is represented in a 5 × 5 supercell). The wave function is expressed as a linear combination of these basis orbitals:

$$|ψ_i⟩ = \sum_α c_α(k)|φ_α(r)⟩$$

The k-dependence of the wave function coefficients is given by Bloch phase factors. We form the perturbed state as:

$$|ψ_i⟩' = |ψ_i⟩ + iqE\sum_{j \neq i} ψ_j \frac{d\psi_j}{dk} |ψ_i⟩ (E_i - E_j)^{-1} |ψ_j⟩$$

where $qE$ is a small parameter.

Given a set of occupied states, the associated density matrix is given by the outer product of the states:

$$ρ = \sum_i f_i |ψ_i⟩⟨ψ_i|$$

The real space density associated with the density matrix is:

$$ρ(k, r) = \sum_{α, β, R, R'} ρ_{α,β}(r - R) φ_α(r) φ_β(r - R') \exp(ik ⋅ (R - R'))$$

RELATION BETWEEN TOTAL DENSITY VERSUS PRIMARY UNIT CELL DENSITY

The density which enters into the relation between velocity and charge density is not the total density, but the density contribution from “on-site” orbitals $ρ_0(r)$. The operator form is as given in the main text:

$$ρ_0(r) = \sum_{M, M'} \left(c_M^† c_{M'} + h.c.\right) φ_M(r) φ_{M'}(r)$$
FIG. 7: Comparison of the total hopping (left side of each subplot) to \( \sigma \)-hopping (right side of each subplot) as a function of the relative orientation (parameterized by polar angles \((\theta, \phi)\)) for all unique pairs of \(d\)-orbitals.

In terms of the density matrix, this quantity is:

\[
\rho_0(\mathbf{r}) = \sum_{\alpha, \beta} \phi_\alpha(\mathbf{r}) \phi_\beta(\mathbf{r})
\]  

(36)

\(\rho_0\) corresponds to only including terms \(\mathbf{R} = \mathbf{R}' = 0\) in Eq. [34]. The charge density in the interstitial regions is quite different for \(\rho(\mathbf{r})\) and \(\rho_0(\mathbf{r})\). However in the vicinity of the nuclei, these densities are quite similar. We show this explicitly in Fig. [8] where we plot \(\delta\rho(\mathbf{r})/qE\) and \(\delta\rho_0(\mathbf{r})/qE\) for applied field in \(x\) and \(y\) directions. As expected, the quantitative difference is quite small near the nuclei. This can be generally anticipated for states with high Berry curvature: Berry curvature is related to the formation of orbital moments, which requires higher values of \(\ell\). These states are more localized than, for example, \(s\)-like states.

**P-ORBITAL MODEL ANALYSIS**

In this section we present a more complete analysis of the \(p\)-model presented in the main text. As described in the main text, \(\sigma\)-hopping leads to \(p_x \leftrightarrow p_x\) and \(p_y \leftrightarrow p_y\) hopping to nearest and 2nd nearest neighbors, and to \(p_x \leftrightarrow p_y\) hopping between second nearest neighbor. The crystal field Hamiltonian in the \((p_x, p_y)\) basis is:

\[
H = \left( \begin{array}{cc}
-2t \cos(k_x) & 4t' \sin(k_x) \sin(k_y) \\
4t' \sin(k_x) \sin(k_y) & -2t \cos(k_y) - 4t' \cos(k_z) \cos(k_y)
\end{array} \right)
\]  

(37)
FIG. 8: Comparison between electric field-induced change of charge density for all charge ($\delta \rho$ of Eq. 34), versus charge only from “on-site” contributions ($\delta \rho_0$ of Eq. 27) for electric fields aligned to the x and y directions. The difference between the two is minimal near atomic centers. Units for all figures are (eV $\cdot$ nm$^2$)$^{-1}$.

The second nearest neighbor hopping $t'$ is related to the first nearest neighbor hopping $t$ as $|t'| = |t|/4$. This relation includes the inter-orbital hopping factor of 1/2 for $p$ orbitals displaced along a 45 degree angle, and the distance-dependence of the hopping given in Eq. 29, which contributes another factor of 1/2.

Re-writing the Hamiltonian given in the main text in terms of radial coordinates for $k = (k_x, k_y) = k (\cos(\theta), \sin(\theta))$, and considering the limit of small $k$, we obtain:

$$H = tk^2 \left( \cos^2(\theta) + \frac{1}{2} \left( \cos(\theta)^2 + \sin(\theta)^2 \right) \right) \left( \sin^2(\theta) + \frac{1}{2} \left( \cos(\theta)^2 + \sin(\theta)^2 \right) \right) + \alpha \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \tag{38}$$

We present the analysis for the response for an applied field along the x-direction, in the limit of $\alpha \ll tk^2$, for a general k point. The unperturbed wave functions are:

$$|\psi_1\rangle = \begin{pmatrix} \cos(\theta) - i\alpha \sin(\theta) \\ \sin(\theta) + i\alpha \cos(\theta) \end{pmatrix} ; \quad |\psi_2\rangle = \begin{pmatrix} -\sin(\theta) - i\alpha \cos(\theta) \\ \cos(\theta) - i\alpha \sin(\theta) \end{pmatrix} \tag{39}$$

The electric field perturbation is $E_x$. Following standard procedures we rewrite the position operator matrix element in terms of $dH/dk_x$:

$$\langle \psi_1|x|\psi_2\rangle = i \frac{\langle \psi_1 | \frac{dH}{dk_x} | \psi_2 \rangle}{E_1 - E_2} \tag{40}$$

The perturbed wave function is then given as:

$$|\psi_1\rangle' = |\psi_1\rangle + i q E \frac{\langle \psi_2 | \frac{dH}{dk_x} | \psi_1 \rangle}{(E_1 - E_2)^2} |\psi_2\rangle \tag{41}$$

$$|\psi_1\rangle' = \begin{pmatrix} \cos(\theta) - i\alpha \sin(\theta) \\ \sin(\theta) + i\alpha \cos(\theta) \end{pmatrix} + \frac{\alpha q E \cos(\theta)}{k^2} \begin{pmatrix} -\sin(\theta) - i\alpha \cos(\theta) \\ \cos(\theta) - i\alpha \sin(\theta) \end{pmatrix} \tag{42}$$
Applying Eq. 6 of the main text leads to the following result for the Berry curvature at a given \(k\) point. See Fig. 9 for definition of vectors \(R_{1,2,3}\) connecting primary unit cell atom to the relevant nearest neighbors.

\[
\Omega_y(k) = 2 \tilde{t} \sigma \left( R_{1,y} \frac{\delta \rho_0^{\text{ang}}(\hat{R}_1)}{E} + R_{2,y} \frac{\delta \rho_0^{\text{ang}}(\hat{R}_2)}{E} + R_{3,y} \frac{\delta \rho_0^{\text{ang}}(\hat{R}_3)}{E} \right)
\]

\[
= 2 \tilde{t} \sigma \left( R_{1,y} a_0 (k_y) + R_{2,y} a_0 (k_x + k_y) + R_{3,y} a_0 (k_x - k_y) \right)
\]

The prefactor of 2 in Eq. 44 accounts for the inversion partners of the three neighbors depicted in Fig. 9. The change in charge density is readily obtained from the perturbed wave function. Writing \(\psi_c = \begin{pmatrix} c_x \\ c_y \end{pmatrix}\), the angular density along the relevant directions are:

\[
\begin{align*}
\frac{\delta \rho_0^{\text{ang}}(\hat{R}_1)}{E} &= |c_y|^2 = -\alpha \left( 2 \sin(\theta) + \sin(3\theta) \right) \\
\frac{\delta \rho_0^{\text{ang}}(\hat{R}_2)}{E} &= \frac{1}{2} \left( |c_x|^2 + |c_y|^2 + 2 \text{Re}(c_x^* c_y) \right) = -\alpha \left( \cos(\theta) + \cos(3\theta) + \sin(\theta) \right) \\
\frac{\delta \rho_0^{\text{ang}}(\hat{R}_3)}{E} &= \frac{1}{2} \left( |c_x|^2 + |c_y|^2 - 2 \text{Re}(c_x^* c_y) \right) = \alpha \left( \cos(\theta) + \cos(3\theta) - \sin(\theta) \right)
\end{align*}
\]

Plugging the expressions for density Eqs. 45 into Eq. 44 leads to the following simple expression for the Berry curvature:

\[
\Omega_y(k) = \frac{4\alpha}{k^4}
\]

Note that \(\Omega\) is independent of the \(\theta\) (the direction of \(k\)) for this model. As expected, Eq. 46 equals the value of \(\Omega\) obtained with direct application of the Kubo formula. Finally, we emphasize that Eq. 9 of the main text does not apply to an arbitrary Hamiltonian; it only applies to Hamiltonians which fully encode the \(\sigma\)-hopping between orbitals on a simple lattice.

### MOS2 Orbital and Real Space Density Analysis

We derive the relation between the electric field-induced charge density integrated over the \(z\)-direction and the Berry curvature of the state at the \(k = \pm K\) points. The spatial integral partially destroys some of the angular dependent information of the density, so that the direction relation Eq. 6 of the main text is no longer directly applicable. However, there is still a relationship between the integrated current and density, as we show next.

To proceed, we write the wave functions of conduction and valence bands (denoted by \(\psi_c\) and \(\psi_v\), respectively);

\[
\begin{align*}
\psi_c(x, y, z) &= A_r \exp \left( -\frac{r}{3a} \right) A_1 \left( -x^2 - y^2 + 2z^2 \right) \\
\psi_v(x, y, z) &= A_r \exp \left( \frac{-r}{3a} \right) \frac{1}{\sqrt{2}} \left( A_2 (xy) + iA_3 (x^2 - y^2) \right)
\end{align*}
\]
where \( r = \sqrt{x^2 + y^2 + z^2} \). The various normalization factors \( A \) are:

\[
A_r = \left( \frac{2}{27} \sqrt{\frac{2}{5}} \left( \frac{1}{3a} \right)^{3/2} \frac{1}{a^2} \right) \tag{49}
\]

\[
A_1 = \frac{1}{4} \sqrt{\frac{5}{\pi}} \quad A_2 = \frac{1}{2} \sqrt{\frac{15}{\pi}} \quad A_3 = \frac{1}{4} \sqrt{\frac{15}{\pi}} \tag{50}
\]

Notice that the radial wave function has a prefactor of \( r^2 \) in the numerator, while the spherical harmonic has a factor of \( r^2 \) in the denominator, the two of which cancel each other.

Consider an applied field in the \( y \)-direction. Upon applying an electric field, we form a linear combination of \( \psi_c \) and \( \psi_v \).

\[
\psi_c' = \psi_c + \left( \frac{i q E t_0}{\Delta^2} \right) \psi_v \tag{51}
\]

The resulting change in density (to lowest order in \( E \) field) is then given as:

\[
\delta \rho(x, y, z) = \left( \frac{2 q E t_0}{\Delta^2} \right) \frac{A_r^2 A_1 A_3}{\sqrt{2}} \exp \left( \frac{-2r}{3a} \right) \left( x^2 - y^2 \right) \left( -x^2 - y^2 + 2z^2 \right) \tag{52}
\]

We focus on \( y = 0 \), so that we have:

\[
\delta \rho(x, 0, z) = \left( \frac{2 q E t_0}{\Delta^2} \right) \frac{A_r^2 A_1 A_3}{\sqrt{2}} \exp \left( \frac{-2\sqrt{x^2 + z^2}}{3a} \right) x^2 \left( -x^2 + 2z^2 \right) \tag{53}
\]

Generally, a two-dimensional map of charge density will involve a convolution function \( f(z) \); its precise form depends on the experiment. For the sake of simplicity, we choose \( f(z) = 1 \) in the analysis presented here. Generalizing to other forms of \( f(z) \) is straightforward, and will result in different numerical prefactors whose precise value is important for quantitative data analysis. Proceeding with \( f(z) = 1 \), we obtain:

\[
\frac{\delta \rho(x)}{E} = \left( \frac{2 q t_0}{\Delta^2} \right) \int dz f(z) A_r^2 A_1 A_3 \exp \left( \frac{-2\sqrt{x^2 + z^2}}{3a} \right) x^2 \left( -x^2 + 2z^2 \right) \tag{54}
\]

To determine the position of the absolute value of the maximum of this function, we first make integral dimensionless with \( z' = z/x \). We also include the numerical prefactors explicitly:

\[
\frac{\delta \rho(x, 0)}{E} = \left( \frac{2 q t_0}{\Delta^2} \right) \left( \frac{1}{27^3} \right)^{1/2} \left( \frac{1}{2 \pi a^2} \right)^{1/2} \int x dx' \exp \left( \frac{-2x'\sqrt{1 + z'^2}}{3a} \right) x^4 \left( -1 + 2z'^2 \right) \tag{56}
\]

Next write \( x \) in dimensionless form, \( x' = x/a \).

\[
\frac{\delta \rho(x', 0)}{E} = \left( \frac{2 q t_0}{\Delta^2} \right) \left[ \left( \frac{1}{27^3} \right)^{1/2} \left( \frac{1}{2 \pi a^2} \right)^{1/2} \int x dx' \exp \left( \frac{-2x'\sqrt{1 + z'^2}}{3} \right) \left( -1 + 2z'^2 \right) \right] \tag{57}
\]

The integral in Eq. 57 must be evaluated numerically for each value of \( x' \). The resulting dimensionless form of the function in brackets is shown in Fig. 10. The position of the maximum of the absolute value is at \( x \approx 8.3a \), and the maximum (absolute) value of the function (in dimensionful form) is \( 1.87 \times 10^{-3} \times \left( \frac{1}{a} \right)^2 \). We combine these two facts to obtain:

\[
\frac{\delta \rho(x_{\text{max}})}{qE} = \left( \frac{2 q t_0}{\Delta^2} \right) 0.128 \times \left( \frac{1}{x_{\text{max}}^2} \right) \tag{58}
\]

Notice that this is quite similar to valley hall conductivity, whose expression is:

\[
\Omega(K) = \frac{2 t^2 a_0^2}{\Delta^2} \tag{59}
\]
FIG. 10: Plot of term in brackets of Eq. 57. The position of the maximum of the absolute value of this curve can be used to estimate the Bohr radius, and the max value of the curve determines the magnitude of the coupling coefficient between \( d_z^2 \) and \( d_{x^2-y^2} \) orbitals. This in turn is related to the magnitude of the Berry curvature.

This enables us to derive a specific relation between the real space properties of the perturbed density and the Berry curvature evaluated at \( \mathbf{K} \):

\[
\Rightarrow \Omega(\mathbf{K}) = 122.07 \times \Delta^2 x_{\text{max}}^4 \left( \frac{\delta \rho(x_{\text{max}})}{qE} \right)^2
\]

(60)

**Energy resolved change in density**

Next we consider the change in the density at a specific energy. To do so we first consider the Berry curvature away from \( \mathbf{k} = \mathbf{K} \). As in the main text, we write the Bloch wave vector as \( \mathbf{q} = \mathbf{k} - \mathbf{K} \), and use polar coordinate for \( \mathbf{q} = (q_x, q_y) = q (\cos(\phi), \sin(\phi)) \). The Hamiltonian is:

\[
H = \begin{pmatrix}
\Delta & tq (\cos(\phi) - i \sin(\phi)) \\
tq (\cos(\phi) + i \sin(\phi)) & -\Delta
\end{pmatrix}
\]

(61)

The Berry curvature is obtained as:

\[
\Omega(q) = 2 \text{ Im} \left( \frac{\langle \psi_c | \frac{dH}{dq} | \psi_v \rangle \langle \psi_v | \frac{dH}{dq} | \psi_c \rangle}{(E_c - E_v)^2} \right)
\]

(62)

\[
= \frac{2a_0^2 t^2 \Delta}{(q^2 t^2 + \Delta^2)^{3/2}}
\]

(63)

To transform this into an energy resolved quantity, we insert a density of states. It’s useful to recall the textbook form of density of states for a (spinless) 2-d system:

\[
D = \frac{Am^*}{2\pi \hbar^2}
\]

(64)

where \( A \) is the unit cell area, \( m^* \) is the effective mass, and \( D \) has units of inverse energy. Note that Eq. 65 assumes a single parabolic band. In the presence of multiple degenerate parabolic bands, \( m^* \) is replaced by the sum of the effective masses of all relevant bands. We focus here on the valence bands, which include bands at \( \pm \mathbf{K} \) and \( \mathbf{k} = 0 \). Only the states near \( \pm \mathbf{K} \) contribute to the Berry curvature, so we find the relevant portion of \( D \) is:

\[
D_K = \frac{Am^*_K}{\pi \hbar^2}
\]

(65)
Note the factor of 2 in the denominator of Eq. 65 is cancelled by a factor of 2 in the numerator owing to the degeneracy of $\mathbf{K}$ and $-\mathbf{K}$.

We next considering the energy resolved absolute value of $\Omega$, (note that the contributions to $\Omega(E)$ from $\mathbf{K}$ and $-\mathbf{K}$ have opposite sign, hence the necessity to consider absolute value of $\Omega$). We obtain:

$$|\Omega(E)| = \frac{A}{(2\pi)^2} \int_{-\pi/a_1}^{\pi/a_1} dk_1 \int_{-\pi/a_2}^{\pi/a_2} dk_2 \delta(E_k - E) \frac{2a_0^2 t^2 \Delta}{(k - K)^2 t^2 + \Delta^2}^{3/2}$$  \hspace{1cm} (66)

$$= \left( \frac{A m_K^*}{\pi \hbar^2} \right) \frac{t^2 \Delta a_0^2}{(2ma_0^2 t^2 E/\hbar^2 + \Delta^2)^{3/2}}$$  \hspace{1cm} (67)

We focus on the small energy limit of Eq. 67 (i.e. energies near the band edges), where $|\Omega(E)|$ is approximately equal to $D_K|\Omega(K)|$. In this limit, similarly the energy-resolved change in density, or local density of states (which we denote by LDOS($E$)) is given by:

$$\frac{\delta \text{LDOS}(E)}{qE} = D_K \frac{\delta \rho(K)}{qE}$$  \hspace{1cm} (68)

Eq. 68 makes the transition from $k$-resolved analysis to $E$ resolved analysis trivial - the two responses are related by the constant factor $D_K$.

Fig. 11 shows the electric field-induced change in the local density of states evaluated at an energy 17 meV below the valence band edge, for fields applied along the $x$ and $y$ directions. (The specific value of energy is not important, as long as it is within 10's of meV near the band edge.) Note that the integration over $z$ has been performed in the data presented here. We find that Eq. 68 is satisfied well in the numerical calculations.

The modification of Eq. 60 for application to change in LDOS is therefore:

$$\Rightarrow \Omega(K) = 122.07 \times \Delta^2 x_{\text{max}}^4 \left( \frac{\delta \text{LDOS}(x_{\text{max}})}{qE} \frac{1}{D_K} \right)^2$$  \hspace{1cm} (69)

Indeed, we find approximate correspondence between computed values and those provided by the estimate of Eq. 69. This shows that, with knowledge of the effective mass of the $K$ valley, the experimental output of an STM experiment may be used to estimate the Berry curvature and valley hall conductivity.
FIG. 11: (a) equilibrium local density of states at an energy 16 meV below valence band edge, integrated over $z$, in units of $(\text{eV} \cdot \text{nm}^2)^{-1}$. (b) and (c) Change in density of this state for field applied along the $x$-direction and $y$-direction, in units of $(\text{eV}^2 \cdot \text{nm})^{-1}$. (d) Linecut of density change through $x$. The distance between atom and maximum in curve is $x_{\text{max}} = 0.07$ nm, the max value of the curve is $0.6 \ (\text{eV}^2 \cdot \text{nm})^{-1}$. 