Anisotropic Magnetoresistance in Multiband Systems: 2DEGs and Polar Metals at Oxide Interfaces

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I. INTRODUCTION

The ability to control the layer-by-layer growth of transition metal oxide heterostructures has led to the discovery and exploration of two-dimensional electron gases (2DEGs) formed at carefully engineered oxide surfaces and interfaces.¹ Such 2DEGs, formed by a combination of a polarization catastrophe² and oxygen vacancies, can combine multiple functionalities of the two bulk quantum materials forming the interface or potentially host new low-dimensional phases of matter. This has led to significant focus on magnetism and superconductivity at the (001) LaAlO₃-SrTiO₃ (LAO-STO) interface.²⁻⁴ Oxide surfaces and interfaces also offer a novel setting to study the role of spin–charge coupling and magnetoelectric effects in 2DEGs.¹⁻² In particular, it has been shown that an electric field can tune the strength of Rashba spin–orbit coupling (SOC) which arises from broken inversion symmetry, permitting control of the Fermi surface (FS) spin-texture and spin–to-charge conversion.⁵⁻⁶ Similarly, an in-plane magnetic field is found to have a significant impact on charge transport, leading to a large negative magnetoresistance in (001) 2DEGs over a range of densities.²建筑师w⁸⁻¹¹ More recent experiments have begun to create and probe 2DEGs at oxide (111) surfaces and interfaces,¹²⁻¹⁰ which have been proposed to host topological phases.¹¹⁻¹⁵

Such (111) interfaces typically lead to more tightly confined 2DEGs.¹⁶⁻¹⁸

Transport experiments on such 2DEGs have studied the anisotropic magnetoresistance (AMR): the change in the diagonal resistivity when the angle between the current direction and the in-plane magnetic field is varied. AMR has also been studied theoretically in the context of spin-dependent impurity scattering on 2DEG samples with finite magnetization and in the context of ferromagnetic semiconductors.¹⁹⁻²³ A useful analysis of the symmetry constraints on the AMR is presented in Ref. ²⁴ These experiments raise the issues of what controls magnetoresistance in multiband systems such as oxide 2DEGs, why their resistance drops when the magnetic fields is rotated from being aligned parallel to the current to being perpendicular to the current direction, and to what extent higher angular harmonics in the AMR directly reflect FS symmetries (e.g., four-fold versus six-fold rotational symmetry of the FS).

Motivated by these questions, we present here a theoretical study of the AMR using a full solution to the semiclassical matrix-Boltzmann equation for the multiband 2DEG with SOC, showing that it captures experimental observations in both (001) and (111) oxide 2DEGs. Focusing on the momentum-dependence of the relevant impurity scattering overlap matrix in the transport equation provides useful insights which are broadly...
applicable to other multiband systems. Our results also suggest that the AMR harmonics do not directly reflect the underlying lattice rotational symmetries of the FS.

For the (001) 2DEG, our work builds upon previous important numerical studies [23-50]. Here, we further suggest simple physical mechanisms for the observations. At zero magnetic field and low density, Fig. 1(a) shows the FSs and the corresponding Rashba spin texture. We find that an effective Rashba SOC enables weak scattering between a ‘circular’ $xy$-orbital dominated band, and an inner ($xz$, $yz$)-orbital dominated ‘propeller’-band. For small SOC, this interband scattering gets suppressed by an in-plane magnetic field leading to large negative magnetoresistance. Changing the angle of the in-plane magnetic field, we find strong angle-dependent current damping and a large AMR, with many angular harmonics at higher fields, as observed experimentally [30] and in previous theoretical work [23-50].

In striking contrast, transport in the (111) 2DEG is dominated by the outermost pair of ‘flower-like’ bands, which arise from strong hybridization of all three $t_{2g}$ orbitals. The corresponding FSs are shown in Fig. 1(b) along with the Rashba spin texture. While the overall resistivity has some contribution from scattering to an inner small ‘hexagon’ band, the angle-dependence of the AMR is dominated by the two large bands. The AMR in this case typically reveals a single $\cos(2\theta)$ angular harmonic. Our results are in qualitative agreement with experimental data [39].

Finally, we explore the impact of directional symmetry-breaking on the (111) 2DEG which leads to a 2D polar metal phase. Such electronic nematicity has been reported in transport experiments [30,39,77]. Polar order in the 2DEG could arise as a result of a bulk structural transition or strong electronic correlations. We argue, within Landau theory, that a polar 2DEG could also arise via a surface phase transition, when the insulating bulk is a paraelectric close to a ferroelectric critical point; this may be of potential relevance to SrTiO$_3$ interfaces. Independent of its microscopic origin, we show that incorporating the nematicity associated with such a polar metal leads to the readily visible violation of some basic symmetry constraints obeyed by the AMR of symmetry-unbroken phases, and also generates higher angular harmonics in the AMR signal. Such simultaneous violations of symmetry constraints and generation of higher harmonics may have been observed in recent experiments at the LAO-STO (111) interface and STO surface.

This paper is organized as follows. We begin with a quick review of the Boltzmann equation for multiband materials, relegating technical details of the computation to Appendix A. We then discuss AMR in the (001) 2DEG and a simplified picture for its origin. We next turn to analogous results for the (111) 2DEG, incorporating the effect of a symmetry-allowed trigonal distortion. Finally, we discuss the impact of directional symmetry breaking on the AMR in (111) 2DEGs in light of recent experimental observations.

II. BOLTZMANN EQUATION

For a weak electric field $\vec{E}$, the semiclassical Boltzmann equation for a multiband system is given by

$$\frac{\partial f_{n,k}}{\partial \epsilon_{n,k}} e^{E_i v^i_{n,k}} = \mathcal{N} \sum_m \int \frac{d^2 k'}{(2\pi)^2} (g_{m,k'} - g_{n,k}) \times |\langle nk|U|m k'\rangle|^2 \delta(\epsilon_{n,k} - \epsilon_{m,k'}),$$

where $f_{n,k}$ and $g_{n,k}$ correspond respectively to equilibrium distribution function and its perturbed non-equilibrium part, labelled by band $n$ and momentum $k$. We use $i$ to denote component indices ($i = x, y$), with implied summation for repeated indices. $\mathcal{N}$ is a constant (proportional to the impurity concentration) which drops out of transport ratio coefficients. The spin-orbit coupled band eigenfunctions, energies, and velocities, are denoted by $|nk\rangle$, $\epsilon_{n,k}$ and $v^i_{n,k}$ respectively; these depend on the magnitude and direction of the applied in-plane magnetic field $\vec{B}$.

The matrix elements for elastic impurity scattering $\langle nk|U|m k'\rangle$ are obtained using a scalar scattering po-
V(k - k')c_{\ell\sigma}^\dagger(k')c_{\ell'\sigma}(k),
\end{equation}

where $V(q) = V_0 e^{-\lambda^2 q^2/4}$. Setting $\Lambda = 0$ corresponds to scattering off a point-like impurity, while $\Lambda \gg a$ (with $a$ being the lattice constant) corresponds to small momentum transfer scattering as appropriate for a smooth real space impurity potential. For SrTiO$_3$, the lattice constant $a \approx 3.9\text{Å}$ is the nearest neighbor Ti-Ti distance in the bulk cubic crystal.

The conductivity tensor within the Boltzmann formalism is then

\begin{equation}
\sigma_{ij} = e^2 \sum_n \int \frac{d^2k}{(2\pi)^2} v_{i,n,k}^* \frac{\partial g_{n,k}}{\partial E^j} . \tag{3}
\end{equation}

Here, $\partial g_{n,k}/\partial E^j$ is computed by taking a derivative of the Boltzmann equation with respect to the electric field, and solving the resulting equations iteratively on a finely discretized momentum mesh in a temperature-dependent window around the FS. The technical details of this approach, including issues related to choice of the momentum mesh and convergence of the solution, are discussed in Appendix A.

The angle-dependent resistivity tensor is calculated by inverting the conductivity tensor $[\rho(\theta)]_{ij} = [\sigma(\theta)^{-1}]_{ij}$. The AMR and its Fourier amplitudes $C_m$ are defined via

\begin{equation}
\text{AMR}(\theta) = \frac{\rho_{xx}(\theta) - \rho_{xx}(|\vec{E}| = 0)}{\rho_{xx}(|\vec{E}| = 0) , \tag{4}
\end{equation}

\begin{equation}
C_m = \int_0^{2\pi} \frac{d\theta}{2\pi} e^{-im\theta} \text{AMR}(\theta) . \tag{5}
\end{equation}

The invariance of the resistivity under $\theta \rightarrow \theta + \pi$ (which is equivalent to flipping the direction of the current) leads to the vanishing of all odd harmonics $C_{2m+1}$, while (mirror) symmetry under $\theta \rightarrow -\theta$ yields purely real Fourier coefficients $C_m$. This latter symmetry is broken for the (111) surface when we include nematic order (see Section V).

III. (001) 2DEG

There have been extensive density functional theory studies of the (001) 2DEG. Experiments have realized the (001) 2DEG at the LaAlO$_3$-SrTiO$_3$ interface, and at SrTiO$_3$ surfaces via photo-doping or Ar ion bombardment. In this last setting, angle-resolved photoemission spectroscopy (ARPES) provides an experimental guide to the FSs of the $t_{2g}$-orbital derived bands. Based on these, and previous work on magnetotransport, we consider the following model.

A. Model Hamiltonian

We begin with the 2DEG square lattice Hamiltonian in the absence of SOC and a magnetic field:

\begin{equation}
H_0^{001} = \sum_{k \sigma \ell \ell'} \epsilon_{\ell \sigma}^\dagger(k) M_{\ell \ell'}^{001}(k) c_{\ell' \sigma}(k) . \tag{6}
\end{equation}

Working in the $\{yz, zx, xy\}$ basis, and using abbreviated notation $s_i \equiv \sin(k_i)$, $c_i \equiv \cos(k_i)$ (with $i = x, y$) we have

\begin{equation}
M_{\ell \ell'}^{001} = \begin{pmatrix} \varepsilon_{yz} & \delta_{xy} & i\zeta_x \\
\delta_{xy} & \varepsilon_{xx} & i\zeta_y \\
-i\zeta_x & -i\zeta_y & \varepsilon_{xy} - \Delta_T \end{pmatrix} , \tag{7}
\end{equation}

where the orbital dispersions are given by

\begin{align}
\varepsilon_{yz} &= 2t_1(1 - c_y) + 2t_2(1 - c_x) , \tag{8} \\
\varepsilon_{xx} &= 2t_1(1 - c_x) + 2t_2(1 - c_y) , \tag{9} \\
\varepsilon_{xy} &= 2t_1(2 - c_x - c_y) . \tag{10}
\end{align}

Here, $t_1$ and $t_2$ are the strong and weak nearest-neighbour intra-orbital hoppings respectively and $\delta_{xy} = 4t_3 g_{x'y'y'}$ is the inter-orbital next-neighbour hybridization. The tetragonal splitting $\Delta_T$ arises from 2D confinement which lowers the $xy$-orbital energy, while the odd-in-momentum inter-orbital hopping $\zeta_i = 2\xi_i$ represents the impact of inversion breaking at the surface.

Finally, the two important terms for the AMR are the atomic SOC and the coupling to the in-plane magnetic field. SOC is captured by the additional term

\begin{equation}
H_{SOC} = \frac{i}{2} \sum_k \epsilon_{\ell m n}^\dagger c_{\ell \sigma}(k) \tau_{n \sigma}^m c_{m \sigma'}(k) , \tag{11}
\end{equation}

(with sums over repeated indices) where $\epsilon_{\ell m n}$ is the Levi-Civita symbol and $\tau^n$ are Pauli matrices. Atomic SOC together with the inversion breaking inter-orbital hopping $\zeta_i$ leads to an effective Rashba SOC. The in-plane magnetic field $\vec{B}$ leads to the term

\begin{equation}
H_B = (g_s \vec{L} + g_s \vec{S}) \cdot \vec{B} , \tag{12}
\end{equation}

with orbital and spin g-factors $g_L, g_s$. Here, the angular momentum components are $L_n = i \sum_k \epsilon_{\ell m n}^\dagger c_{\ell \sigma}(k) c_{m \sigma'}(k)$.

For a quantitative study of the 2DEG, we follow Ref. [23] and fix $(t_1, t_2, t_3, \Delta_T, \zeta, \lambda) \equiv (340, 13, 6, 60, 8, 5)\text{meV}$. We set the orbital $g$-factor to be $g_L = 1$, and the spin $g$-factor to be $g_s = 5$, with $g_s > 2$ chosen to mimic enhanced ferromagnetic correlations observed in certain such 2DEGs. The transport properties for this system are calculated as a function of the angle $\theta$ between the in-plane $\vec{B}$ field and the current (which we assume to run along the [100] crystal axis).
The zero field FS for the Hamiltonian \( H^{001}_0 + H_{SOC} \) is shown in Fig. 1(a) for \( n = 0.035 \) electrons per Ti, with colors indicating the orbital content. We also show the corresponding spin texture on each band (with a different color arrow for spin chirality), from which the opposite chirality on pairs of effective Rashba bands is clearly visible. We observe four FSs; the outer two FSs have dominant \( xy \)-character, with some \( zz\)-character near the \( k_z = 0 \) and \( k_y = 0 \) directions, while the inner two FSs have dominant \( zz\)-character.

Fig. 2(a) shows the calculated AMR signal (blue curve) as a function of magnetic field angle \( \vartheta \), with current along the [100] direction, for \( |\mathbf{B}| = 20T \), temperature \( T = 10K \), and impurity scattering length \( \Lambda = 5a \). We highlight a few observations from these results: (i) The angle averaged value of the AMR signal indicates a large negative MR as observed in the experiments. (ii) We find that resistivity is significantly lower for fields perpendicular to the current. (iii) From the Fourier modes plotted in Fig. 2(b), we find several nonzero harmonics reflecting the complexity of the AMR signal.

In order to obtain a simple understanding of these results, we have carried out a detailed analysis to see which bands dominate the AMR. Labelling the four bands as \( n = 1, 2, 3, 4 \) from the largest to the smallest, we find that the AMR mostly arises from a single pair of bands: the ‘circular’ band-2 and the ‘propeller’ band-3. We show the AMR and its harmonic decomposition calculated by projecting to just these two bands in red in Fig. 2(a) and (b). In this simplified calculation, we diagonalize the full Hamiltonian for the band wavefunctions and energies, but retain just the two coupled bands in solving the Boltzmann equation. We see that this two-band system semi-quantitatively captures the AMR and its harmonics. To see why this simplified two-band scenario works well, we observe that the outer two bands, derived largely from the \( xy \) orbitals, are expected to dominate the diagonal conductivity of the system since they have a larger Fermi surface and a higher Fermi velocity compared with the quasi-1D inner bands. For impurity scattering with small momentum transfer, we also see that intra-band scattering will not efficiently degrade the current carried by these bands since it will mostly lead to forward scattering. Thus, the transport lifetime of these bands is limited by inter-band scattering. Indeed, scattering to the inner ‘propeller bands’ provides an extremely efficient way to degrade current since these bands have a smaller Fermi velocity, and a FS shape which results in their Fermi velocity mostly pointing away from \( \hat{x} \).

Fig. 3(a)-(c) shows the Fermi surface for \( \vartheta = 0, \pi/4, \pi/2 \). From the spin textures on the FSs, it is clear that the outermost band-1 can continue to scatter strongly to the inner ‘propeller’ band-3 whose shape permits efficient current decay. Thus, band-1 does not have its conduction significantly altered by the magnetic field. However, at this magnetic field, band-2 has its spin nearly antiparallel to the inner band-3 at any field angle while the spins were parallel at zero field (Fig. 1(a)), so any impurity-induced interband scattering to the inner band is strongly suppressed by applying a field. This leads to a magnetic field induced enhancement of transport lifetime for band-2, and a concomitant large negative magnetoresistance.

To further analyze the angle-dependence of the AMR, we plot in Fig. 3(a)-(c) the impurity scattering overlap matrix \( \langle n\mathbf{k}|U|n\mathbf{k}'\rangle^2 \delta(\varepsilon_{n,\mathbf{k}} - \varepsilon_{m,\mathbf{k}'}), \) keeping a fixed momentum \( \mathbf{k} \) on band-2 indicated by the blue cross (which is the current-carrying region), and for varying momentum \( \mathbf{k}' \) on band \( m = 3 \). For \( \vartheta = 0 \) as in Fig. 3(a), we see that the dominant scattering occurs to the forward elongated ellipse part of band-3, which has its Fermi velocity typically directed away from \( \hat{x} \), so the resulting transport lifetime will be short. Carriers preferably scatter to this region of the FS because it is closer to the initial momentum which satisfies the small-momentum transferring potential, and the spins are not full antiparallel with the spin at \( \mathbf{k} \) (marked with the blue ×). However, when \( \vartheta = \pi/2 \) as in Fig. 3(c), the scattering occurs into the vertical ellipse part of band-3, which has its Fermi velocity along \( \hat{x} \), leading to less efficient current decay, resulting in a longer transport lifetime. This portion of Fermi momenta is preferred because the previously

![AMR and Fourier modes](image-url)
favored region in the horizontal ellipse now has a fully antiparallel spin with the spin at \( k \). Since the momentum transfer between \( k \) and the vertical ellipse is large, the scattering potential suppresses this scattering channel which explains the small overlap matrix as seen from the colorbar. Thus, we expect the resistivity to be much lower for \( \vartheta = \pi/2 \). The reason the spins are not fully parallel or antiparallel stems from the competition between the Rashba energy scale which becomes important for large Fermi momenta and the magnetic field energy scale. A simple model which captures this behavior is provided in Appendix C. If the \( \vartheta \)-dependence of this overlap pattern was smooth, we would expect a single \( \cos(2\vartheta) \) harmonic in the AMR; however, the pattern at \( \vartheta = \pi/4 \) (see Fig. 3(b)) is nearly the same as for \( \vartheta = 0 \), so the pattern changes abruptly with angle for \( \vartheta > \pi/4 \), resulting in many harmonics \( \cos(2m\vartheta) \) in the AMR. In particular, the AMR has \( \cos(6\vartheta) \) components which are symmetry allowed harmonics although the FS itself does not have six-fold symmetry.

IV. (111) 2DEG

The (111) 2DEG at oxide surfaces and interfaces has also been studied using ARPES. Based on such experiments, we can write a general \( 6 \times 6 \) Hamiltonian and fit hopping parameters to qualitatively reproduce the shape of the Fermi surfaces seen in experiments.

A. Model Hamiltonian

We begin with the zero field Hamiltonian

\[
H_0^{111} = \sum_{k \sigma \ell' \ell} \epsilon_{\ell' \sigma}^\dagger(k) M_{\ell' \ell}^{111}(k) c_{\ell' \sigma}(k),
\]
defined on a triangular lattice, where

\[ M^{(111)} = \begin{pmatrix}
\varepsilon_{yz} & \gamma_a + i\delta_b - \frac{2\Delta}{3} & \gamma_b - i\delta_c - \frac{2\Delta}{3} \\
\gamma_a - i\delta_b - \frac{2\Delta}{3} & \varepsilon_{xx} & \gamma_c + i\delta_a - \frac{2\Delta}{3} \\
\gamma_b + i\delta_c - \frac{2\Delta}{3} & \gamma_c - i\delta_a - \frac{2\Delta}{3} & \varepsilon_{xy}
\end{pmatrix} \] (14)

Similar to the (001) case, we use the abbreviated notation \( c_i, s_i \), with \( \hat{i} = \hat{a}, \hat{b}, \hat{c} \), where \( \hat{a} = \hat{x}, \hat{b} = -\hat{x}/2 - \hat{y}\sqrt{3}/2, \) and \( \hat{c} = -\hat{x}/2 + \hat{y}\sqrt{3}/2 \). With this notation, the intra-orbital dispersions are

\[ \varepsilon_{yz} = 2t_1(1 - c_e) + 2t_2(2 - c_a - c_b), \]

\[ \varepsilon_{xx} = 2t_1(1 - c_b) + 2t_2(2 - c_a - c_c), \]

\[ \varepsilon_{xy} = 2t_1(1 - c_c) + 2t_2(2 - c_b - c_c), \] (15) (16) (17)

while the inter-orbital hybridization \( \gamma_i \equiv -2t_3c_i \), the odd-in-momentum term \( \zeta_{ij} = 2\zeta(s_i + s_j) \) represents hopping permitted by broken inversion symmetry at the interface, and \( \Delta \) is a symmetry-allowed trigonal distortion term. This Hamiltonian is again supplemented with \( H_{SO} + H_B \) as for the (001) 2DEG.

The ARPES data on the STO (111) surface is reasonably fit by choosing \( (t_1, t_2, t_3) = (320, 13, -13) \)meV. In addition, for simplicity, we pick \( (\zeta, \lambda) \equiv (8, 5) \)meV as for the (001) 2DEG. We also use the same g-factors \( g_e = 1 \) and \( g_s = 5 \) for coupling to the in-plane \( B \) field, with the field angle \( \vartheta \) being defined with respect to the \([-110]\) crystal axis.

We have explored several values of the symmetry-allowed trigonal distortion scale \( \Delta \) as shown in Fig. 3. We find that the AMR is reasonably described using values of \( \Delta \approx 50 - 80 \)meV, which are similar to the scale of \( \Delta_T = 60 \)meV in the (001) 2DEG. It is important to note that this local distortion energy scale is different from the band degeneracy splitting at the \( \Gamma \)-point of the BZ; this is given by \( 6t_3 + \Delta \) for the (111) 2DEG, unlike the (001) case where it is just \( \Delta_T \). Furthermore, it has been recently pointed out that this scale can be density-dependent due to renormalization by electron-electron interactions. Here, for simplicity, we focus on a single density \( n = 0.05e/Ti \), and view \( \Delta \) as the renormalized distortion.

B. Magnetotransport

For \( n = 0.05e/Ti \) and \( \Delta = 70 \)meV, the (111) 2DEG exhibits four Fermi surfaces with Rashba-like spin textures as shown in Fig. 1(b). The calculated AMR signal for this case is shown as the blue curve in Fig. 4. We find that the magnitude of the angle-averaged MR is smaller than for the (001) case, but it is tunable by changing the trigonal distortion \( \Delta \) as seen from Fig. 5. In all cases, we find that the AMR has \( C_2 \) character, with no sign of higher harmonics. This is qualitatively consistent with experimental observations. We have found that this \( C_2 \) dominant response, with almost no sign of higher harmonics, holds true even up to much higher densities \( n \sim 0.4e/Ti \).

To understand the average MR, we plot the spin texture on the FSs in Fig. 3 at nonzero \( B \), which shows that there is a significant contrast with the (001) 2DEG — namely, the outer pair of bands features opposite spin polarizations, and so does the inner pair of bands. As a result, each outer band (band-1 or band-2) has a corresponding inner band (band-3 or band-4) into which it can scatter even when \( \vec{B} \neq 0 \); this leads to a reduced MR, since no scattering channel is “switched off” by the...
field unlike in the (001) 2DEG. The tunability of the MR with $\Delta$ arises due to changes in the FS spin textures, such that an inner band flips its spin polarization; the mechanism for large negative MR then parallels that of the (001) 2DEG.

The sign of the $C_2$ harmonic in the AMR may be understood from the overlap matrix plots in Fig. 6. It is clear that both $\vartheta = 0$ and $\vartheta = \pi/2$ have scattering from the marked blue cross on band-1 to momenta on band-2 where the Fermi velocity points away from $\hat{x}$, leading to current dissipation. However, the magnitude of this overlap is smaller for $\vartheta = \pi/2$ (see color scale), which suppresses the resistivity for this field angle.

We attribute the absence of higher harmonics in the AMR signal to the fact that each band in the (111) 2DEG has an equal (momentum dependent) mixture of all three orbitals $yz, zx, xy$, which independently have strong directional character. This is different from the (001) 2DEG where the more unidirectional $yz, zx$ orbitals are split off from the symmetric $xy$ orbitals.

V. IMPACT OF SYMMETRY BREAKING IN THE (111) 2DEG: A 2D POLAR METAL

We turn next to the question of how directional symmetry breaking at the (111) interface, which leads to a 2D polar metal phase, might impact the AMR in the 2DEG. Our work is partly motivated by experimental reports of nematicity in transport measurements in such 2DEGs.\cite{43,44,45} Such symmetry breaking might have its origin in the bulk 3D structure; e.g., bulk SrTiO$_3$ has a structural cubic-to-tetragonal transition upon lowering temperature.\cite{46} $T \lesssim 100$K. If the tetragonal domains are aligned, it will impose a nematic distortion for 2DEGs at the surface or interface of such a crystal. In high density 2DEGs, symmetry breaking may also be driven by electron interaction,\cite{47} which can lead to orbital-ordering or cause a Pomeranchuk instability of the FS. Finally, as discussed in the introduction, the surface or interface hosting the 2DEG might undergo a surface phase transition, leading to a polar metal breaking discrete rotational and mirror symmetries of the 2DEG.

A. Landau theory and coupling to electrons

Independent of its microscopic origin, the order parameter for such a nematic in (111) 2DEGs is a complex
scalar \( \psi \), with the Landau theory taking the form
\[
F_{111} = \frac{1}{2} |\psi|^2 + w(\psi^3 + \psi^\dagger^3) + u|\psi|^4 + \ldots,
\]
where cubic terms lead to an effective \( Z_3 \) clock model.
A similar model has been studied long ago for bulk SrTiO\(_3\) in the presence of a stress applied along the (111) direction\(^{[22]}\). We present a heuristic derivation of this in Appendix \([3]\) discussing its relation to the proximity of SrTiO\(_3\) to a paraelectric-ferroelectric quantum phase transition.

The impact of this symmetry breaking is captured by a local linear-in-\( \psi \) coupling to the orbitals via
\[
H_\psi = -\frac{1}{2} \hat{v}_1 \left[ (L_x^2 + \omega L_y^2 + \omega^2 L_z^2) \psi + \text{h.c.} \right] - \frac{1}{2} \hat{v}_2 \left[ (L_y L_x + \omega L_z L_x + \omega^2 L_x L_y) \psi + \text{h.c.} \right],
\]
where \( \omega = e^{2\pi i/3} \), and we have defined the symmetrized product \( L_i L_j \) by \( L_i L_j = L_i L_j + L_j L_i \). Explicitly, this leads to an orbital Hamiltonian
\[
H_\psi = \begin{pmatrix}
    v_1 \cos(\chi) & v_2 \cos(\chi + \frac{2\pi}{3}) & v_2 \cos(\chi + \frac{2\pi}{3}) \\
    v_2 \cos(\chi + \frac{2\pi}{3}) & v_1 \cos(\chi + \frac{2\pi}{3}) & v_2 \cos(\chi) \\
    v_2 \cos(\chi + \frac{2\pi}{3}) & v_2 \cos(\chi) & v_1 \cos(\chi + \frac{2\pi}{3})
\end{pmatrix}.
\]

The resulting distorted FSs and their spin textures are shown in Fig. 7 at two different densities \( n = 0.05e/Ti \) and \( n = 0.2e/Ti \). For illustrative purposes, we have chosen \( v_1 = v_2 = -11\text{meV} \) and \( \chi = \pi \). We find that the observed distortion of the FS is harder to resolve at higher densities where ARPES studies\(^{[32]}\) have been carried out on the (111) surface 2DEG of SrTiO\(_3\).

**B. Magnetotransport**

The AMR in the presence of this symmetry breaking field, with \( v_1 = v_2 = -11\text{meV} \) and \( \chi = \pi \), is shown in Fig. 8. We find that the AMR exhibits several new aspects absent in the symmetric 2DEG: (i) The AMR is no longer symmetric under \( \vartheta \to -\vartheta \), which allows for sinusoidal components in the Fourier decomposition. (ii) We find higher angular harmonics being generated by the symmetry breaking. These observations appear consistent with experiments\(^{[32]}\), where the onset of higher \( C_6 \) harmonics in the AMR appears to coincide with the breaking of the \( \vartheta \to -\vartheta \) symmetry of the signal, suggesting that these two phenomena go hand in hand, and might be tied to directional symmetry breaking in the 2DEG. As shown in Fig. 8, all of these results including the correct sign of the Fourier modes, can be qualitatively reproduced by keeping just a single pair of bands in solving the Boltzmann equation. Unlike the non-symmetry broken phase discussed previously, the relevant bands are now bands 1 and 4 which have different shapes and orbital content – the outermost band is mainly composed of \( xz, zx \) orbitals while the innermost band has a predominant \( yz \) character. This situation is similar to the (001) calculation where the relevant bands 2 and 3 had different geometries/orbital contents leading us to believe that this orbital imbalance and different geometry could be responsible for the generation of higher harmonics.

**VI. SUMMARY AND DISCUSSION**

We have considered model 2D Hamiltonians for both (001) and (111) oxide interfaces, and obtained insights into their magnetotransport properties by solving the full matrix Boltzmann equation and studying the momentum dependence of the scattering overlap matrix. We have also shown that simplified two-band solutions
to the Boltzmann equation can qualitatively capture many of these features. We summarize below some of the key results and discuss some speculative ideas:

(i) We have shown that the MR and its angle dependence appear to be governed by the field-dependent tuning of interband scattering.

(ii) Octahedral distortions, such as the trigonal distortion at the (111) interface, can significantly affect the FSs and MR, suggesting that engineering or tuning such distortions may provide a viable route to controlling transport properties of such 2DEGs.

(iii) We have argued, and provided a Landau theory reasoning, for why (111) oxide interfaces might stabilize polar metal phases, particularly those involving SrTiO$_3$ which are proximate to a bulk ferroelectric critical point. Our work suggests that the AMR and its symmetries may be used to indirectly detect such symmetry breaking. Furthermore, the nematic resistivity observed in insulating ultra-low density (111) 2DEGs may be viewed as arising from an “Anderson-localized polar metal” which exhibits anisotropic variable-range hopping. It would be interesting to further explore this regime.

(iv) While the dominant AMR mode is the uniform $C_2$ angular component, we have shown that higher harmonics can emerge in symmetric (001) 2DEGs and in nematic/polar (111) 2DEGs. In particular, the higher AMR harmonics appear not to be directly related to FS symmetries. However, a common emerging picture, based on comparing the (001) and (111) 2DEGs, is that these harmonics may arise from a shape mismatch between the two bands which govern the AMR.

(v) Finally, various experiments on the metallic (111) 2DEGs report a change in the AMR when cooling below $T^* \lesssim 20-25\text{K}$ which depends on density and is consistent with underlying polar symmetry breaking. This may reflect the actual symmetry breaking temperature scale of the 2DEG, or might reflect a temperature at which the 2DEG effectively “approaches” the symmetry-broken interface, with the polar order onset already occurring at a higher transition temperature. Future studies of this issue would be valuable.

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where we have dropped factors of \( N, e \) since we will only be interested in ratios of transport coefficients where these will cancel. Taking a derivative with respect to \( E^i \), and lumping together band and momentum indices via \( \mu \equiv (n, k), \nu \equiv (m, k') \) we get
\[
\left( -\frac{\partial f}{\partial \varepsilon^i} \right)_{\mu} = \sum_{\nu, \alpha} (\delta_{\alpha \mu} - \delta_{\alpha \nu}) |U_{\mu \nu}|^2 \delta(\varepsilon_\mu - \varepsilon_\nu) \left( \frac{\partial g}{\partial E^i} \right)_{\alpha},
\]
where \( U_{\mu \nu} = \langle \mu | \hat{U} | \nu \rangle \), \( B_{\mu \alpha} = \langle \mu | \hat{U} | \alpha \rangle |^2 \delta(\varepsilon_\mu - \varepsilon_\alpha) \) and \( A_{\mu \alpha} \equiv \sum_{\nu} B_{\mu \nu} \delta_{\alpha \nu} \). Equation (A2) is a matrix inversion problem for the ‘vector’ \( (\partial g/\partial E^i) \); however \((A - B)^{-1}\) is not well defined since it has a zero eigenvalue associated with a constant (band and momentum independent) vector \((\partial g/\partial E^i) \propto 1\). Rather than using SVD algorithms and pseudoinverse techniques, we found that an efficient way to solve Eq. (A2) is to write it as an iterative equation
\[
\left[ \frac{\partial g}{\partial E^i} \right]_{p+1} = A^{-1} \left( B \cdot \left[ \frac{\partial g}{\partial E^i} \right]_p - \frac{\partial f}{\partial \varepsilon^i} \right).
\]
We begin at step \( p = 0 \) by guessing a random initial vector \( [\partial g/\partial E^i]_{p=0} \), removing its projection in the constant eigenvector subspace, and evaluating the r.h.s. of the above equation to obtain a new \( [\partial g/\partial E^i]_{p=1} \). We then repeat this process, taking care at each step to remove the projection of \( [\partial g/\partial E^i]_p \) to the constant eigenvector (to avoid errors which can creep in from numerical precision). Convergence is reached when the \( L_2 \) norm \( \| \frac{\partial f}{\partial \varepsilon^i} + (A - B) \frac{\partial g}{\partial E^i} \| < \text{tol} \), where tol is typically chosen to be \( 10^{-10} \).

We find that for proper convergence one must choose momentum mesh sizes of the order 2500 \( \times \) 2500 for temperatures of \( T \sim 5K \). Since the \((A, B)\) matrix dimensions scales as \( (6 \times 2500^2) \times (6 \times 2500^2) \) for a 6-band problem, the memory requirements far exceed what can be handled by clusters. In order to reduce the dimensionality of the problem, we use the fact that \( g \) and \( \partial g/\partial E^i \) must go to zero far from the Fermi momenta and work with momenta within a certain temperature \( T \) window of the Fermi momenta. It is found that a temperature window of \( \pm 6 \times T \) is reasonable for low densities \((n \lesssim 0.1)\) while one needs up to \( \pm 12 \times T \) at high densities \( n \gtrsim 0.4 \).

### Appendix B: Landau theory of nematic/polar 2DEG

We start with the Landau theory for ferroelectric order in a bulk 3D cubic crystal in terms of the vector order parameter \( \vec{\phi} = (\varphi_x, \varphi_y, \varphi_z) \) which represents the electric dipole moment due to off-center displacement of Ti atom within the oxygen octahedra in materials like BaTiO\(_3\) or SrTiO\(_3\). The \((x, y, z)\) components refer to cubic axes of crystal. The symmetry allowed bulk terms are
\[
\mathcal{F}_{\text{bulk}} = r_B \vec{\phi}^2 + u_B \varphi_x^4 + u_y \varphi_y^4 + u_z \varphi_z^4,
\]
with subscript \( B \) on the coefficients denoting bulk. Explicit spatio-temporal gradients of the order parameter, stemming from thermal or quantum fluctuation effects are ignored here; they are only taken into account to the extent that they renormalize the coefficients of this effective Landau theory. Here, \( r_B \propto (T - T_c) \) where \( T_c \) is the mean field ordering temperature into the 3D ferroelectric state. Since SrTiO\(_3\) remains a paraelectric, it has \( r_B > 0 \) down to the lowest temperature, but proximity to a quantum critical point can lead to small \( r_B(T = 0) \). Even in such cases, where the bulk remains a paraelectric, a spontaneous symmetry breaking state might still arise at the surface.

With \( \vec{n} \parallel [111] \), additional terms are allowed at the surface,
\[
\Delta \mathcal{F}_{111} = \alpha \varphi \cdot \vec{n} + g (\vec{\varphi} \cdot \vec{n})^2 + \lambda_1 (\vec{\varphi} \cdot \vec{n})^3 + \lambda_2 (\vec{\varphi} \cdot \vec{n}) \varphi_x^2 + \lambda_3 \varphi_x \varphi_y \varphi_z + w_1 (\vec{\varphi} \cdot \vec{n})^4 + w_2 (\vec{\varphi} \cdot \vec{n})^2 \varphi_x^2 + w_3 (\varphi_x^2 \varphi_y + \varphi_y^2 \varphi_z + \varphi_z \varphi_x^2). \]
From the bulk free energy, \( w_B < 0 \) favors states where the dipole moment points along [100] or symmetry related axes for a total of 6 symmetry related ground states. At a (111) surface, the inversion breaking term \( \alpha \) splits this 6-fold degeneracy into two triplets \((+\hat{x}, +\hat{y}, +\hat{z})\) and \((-\hat{x}, -\hat{y}, -\hat{z})\). Any symmetry breaking surface phase transitions will involve breaking the residual \( C_3 \) and mirror symmetries of these triplets.

Similarly, \( w_B > 0 \) in the bulk free energy favors the eight degenerate states where the dipole moment points along [111] and its symmetry equivalents. At the (111) surface, \( g > 0 \) breaks this degeneracy into a high energy doublet (with dipoles along \( \pm \hat{n} \)) and a low energy sextet with dipoles along the other directions: \((1\bar{1}1), \bar{1}(111), (11\bar{1}), (\bar{1}1\bar{1}), \) and \((\bar{1}\bar{1}1)\). The term \( u \) of such a Landau theory in Fig. 9. Here, we choose to include the in-plane spontaneous symmetry breaking order parameter \( \bar{\sigma} = 1, \) we set \( r_B = 0.01, \) and we vary \( w_B. \) For the surface coefficients, we set \( \alpha = -0.2, \lambda_1 = \lambda_2 = 0 \) and drop quartic invariants \( w_1 = w_2 = w_3 = 0 \) while varying \( g = \lambda_3. \) Since the surface breaks \( \hat{n} \rightarrow -\hat{n} \) inversion, it is useful to parametrize

\[
\bar{\psi} \equiv \varphi_{\parallel} \hat{n} + \psi \hat{\gamma} + \psi^* \hat{\gamma}^*,
\]

where \( \hat{n} \equiv (1, 1, 1)/\sqrt{3}, \) \( \hat{\gamma} \equiv (1, \omega, \omega^2)/\sqrt{3}, \) and \( \omega = e^{2\pi i/3}. \) Here, \( \varphi_{\parallel} \) is a non-symmetry-breaking polarization, while the complex \( \psi \neq 0 \) reflects spontaneous symmetry breaking of the surface symmetries.

As an illustrative example, we plot the phase diagram of such a Landau theory in Fig. 9. Here, we choose to work in units where the bulk Landau theory coefficient \( u_B = 1, \) we set \( r_B = 0.01, \) and we vary \( w_B. \) For the surface coefficients, we set \( \alpha = -0.2, \lambda_1 = \lambda_2 = 0 \) and drop quartic invariants \( w_1 = w_2 = w_3 = 0 \) while varying \( g = \lambda_3. \) Since the surface breaks \( \hat{n} \rightarrow -\hat{n} \) inversion, it is useful to parametrize

\[
\bar{\psi} \equiv \varphi_{\parallel} \hat{n} + \psi \hat{\gamma} + \psi^* \hat{\gamma}*,
\]

where \( \hat{n} \equiv (1, 1, 1)/\sqrt{3}, \) \( \hat{\gamma} \equiv (1, \omega, \omega^2)/\sqrt{3}, \) and \( \omega = e^{2\pi i/3}. \) Here, \( \varphi_{\parallel} \) is a non-symmetry-breaking polarization, while the complex \( \psi \neq 0 \) reflects spontaneous symmetry breaking of the surface symmetries.

We can simplify the Landau theory to focus only on the in-plane spontaneous symmetry breaking order parameter \( \psi. \) Substituting the above expression in the free energy \( \mathcal{F} + \Delta \mathcal{F}_{111}, \) we arrive at the simplified free energy at the (111) surface

\[
\mathcal{F}_{111} = r|\psi|^2 + w(\psi^3 + \psi^*3) + u|\psi|^4 + \ldots, \tag{B4}
\]

used in the main text. In the absence of conduction electrons, the state with \( \psi \neq 0 \) is a nematic which breaks rotational symmetry. Due to the symmetry-allowed cubic term \( w \) which breaks \( \psi \rightarrow -\psi \) symmetry, it is also a surface ferroelectric with an in-plane ferroelectric moment. The conducting 2DEG at the surface will convert this into a “polar metal” phase which exhibits nematic transport.

**Appendix C: Two-band model**

In order to get some insight about the sign of the \( C_2 \) Fourier coefficient, we consider the following Hamiltonian in the \(|\uparrow\rangle, |\downarrow\rangle\) basis, with a continuum Rashba term and a Zeeman field:

\[
H(k) = \varepsilon_k^0 \sigma_0 + \lambda(\sigma \times k) \cdot \hat{\nu} + \hat{\nu} \hat{B} \cdot \sigma. \tag{C1}
\]

The eigenvalues and eigenvectors are given by:

\[
\varepsilon_{k,\pm} = \varepsilon_k^0 \pm \sqrt{\lambda^2|k|^2 + g^2|\hat{B}|^2 + 2\lambda g(k_y B_x - k_x B_y)}, \tag{C2}
\]

\[
|u_\pm(k)\rangle = \frac{1}{\sqrt{2}}(\pm e^{i\phi_k}, 1)^T, \tag{C3}
\]

where \( \tan(\phi_k) \equiv \left(\frac{\lambda k_x - g B_y}{\lambda k_y + g B_x}\right). \) At a given electronic density, one can calculate the overlaps between points \( k \) and \( k + \delta k \) both sitting at the Fermi level of two bands with different chirality. For a scalar scattering potential we can only focus on the eigenstates overlaps:

\[
|\langle u_\pm(k + \delta k)|u_\mp(k)\rangle|^2 = \sin^2\left(\frac{\phi_k + \delta \phi_k - \phi_k}{2}\right), \tag{C4}
\]

\[
|\langle u_\pm(k + \delta k)|u_\pm(k)\rangle|^2 = \cos^2\left(\frac{\phi_k + \delta \phi_k - \phi_k}{2}\right). \tag{C5}
\]

Parameterizing the in-plane components in polar coordinates via \( \hat{B} = |\hat{B}|(\cos \vartheta, \sin \vartheta), k = |k|(\cos \alpha, \sin \alpha), \)
\( \delta k = |\delta k| (\cos \beta, \sin \beta) \) and rescaling \( g = g' |\vec{B}| \), we can expand to leading order in \( \lambda/g \) (large magnetic field limit) and \( g/\lambda \) (large Rashba limit):

\[
|\langle u_\pm (k + \delta k)|u_\mp (k) \rangle|^2 \approx \frac{\lambda^2}{4g^2} \cos^2(\beta - \vartheta) + O\left( \left( \frac{\lambda}{g} \right)^3 \right), \quad \text{(C6)}
\]

\[
|\langle u_\pm (k + \delta k)|u_\mp (k) \rangle|^2 \approx \sin^2\left( \frac{\alpha - \beta}{2} \right) + O\left( \frac{g}{\lambda} \right). \quad \text{(C7)}
\]

From this, it is clear that in the large field limit the overlap is minimal for \( \beta = \vartheta \pm \frac{\pi}{2} \) and its maximum is when \( \beta = \{\vartheta, \vartheta \pm \pi\} \), independently of the position of \( k \). In other words, the spins on each band will either align or anti-align with the magnetic field. In the large Rashba limit we distinguish two cases: (i) For \( |\delta k| > |k| \) the overlap is maximized when \( \beta = \alpha \pm \pi \), and (ii) For \( |\delta k| < |k| \) it is maximized for \( \beta = \alpha \pm \cos^{-1}\left(-|\delta k|/|k|\right) \).

The details of this will be determined by the explicit shape of the scattering potential and the scattering lengthscale. For a point at \( k_y = 0 \), i.e. \( \alpha = 0 \) like those considered in Figs. 3 and 6, the two overlaps (C6) and (C7) can be simultaneously maximized for a field in the \( x \)-direction by choosing \( \beta = \pm \pi \) leading to an overall higher resistivity. On the other hand, for a field pointing in the \( y \) direction no choice of \( \beta \) can maximize the two overlaps, giving rise to a competition between the Rashba and magnetic field energy scales and thus reducing the total overlap and resistivity.