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2 Semiclassical theory of anisotropic transport at LaAlO$_3$ / SrTiO$_3$ interfaces

2.1 Introduction

The development of quantum-matter heterostructures paves the way to the realization of novel electronic states, due to the combination of the capabilities and rich variety of heterostructure engineering, the collective interactions of complex oxides, and the emergent properties of quantum materials [82, 83].

A paradigmatic example is the heterostructure formed by the transition-metal oxides LaAlO$_3$ and SrTiO$_3$. Since the experimental demonstration of electrical conduction at the interface between these two materials [23], large attention has been drawn to this system in particular due to its gate-tunable superconductivity [33, 34, 84] at $T \lesssim 300$ mK. At slightly higher temperatures — in the range $1 - 20$ K — magnetotransport has been an important tool for the investigation of electronic and magnetic properties of the interface that are believed to be strongly determined by mixing of charge, spin, orbital and lattice degrees of freedoms.

A number of signatures in the normal-state transport [49, 50, 85, 86], such as giant negative magnetoresistance, crystalline anisotropy, anomalous Hall effect and their striking change of behavior when the system is tuned across a Lifshitz transition [36] have been considered as an evidence of magnetism at the interface. In particular, Ruhman et al. [48] suggested that the action of the field on the interaction between conduction electrons and localized magnetic moments induces a phase transition from a Kondo-screened (high and isotropic resistance) phase to a (low and anisotropic resistance) polarized phase, where the unscreened moments act as magnetic scatterers.

However, experimental investigations of the magnetic landscape at the interface [30, 42, 43, 87–89] reported qualitatively different results. A strong ferromagnetic phase with large total magnetization was recently
observed by magnetic force microscopy [46] at room-temperature in the depleted (insulating) regime of top-gated interfaces. On the other hand, the total magnetization was found to disappear when the interface was doped enough to be conducting. More questions about the origin and the nature of magnetism at low temperature remain to be answered.

A particular type of spin-orbit coupling at the interface is produced by the interplay of atomic spin-orbit interaction (intrinsic to \(d\) electrons) and the next-nearest-neighbour hopping from \(d_{xy}\) to \(d_{xz}/d_{yz}\) orbitals, a process that is forbidden in the bulk due to inversion symmetry, but it is activated at the interface. Spin-splitting without magnetic field has been experimentally measured: the magnitude of the splitting is strongly dependent on the position of the Fermi level (tuned via external gate-voltage) and seems to increase steeply in the overdoped regime [35, 84, 90]. Motivated by the experimental observations, models including tunable spin-orbit coupling through an explicit density-dependence of the parameters have been applied to study thermodynamic properties of the interface, pointing out the possibility of realizing electronic phase separation in a self-consistent manner [91, 92]. Furthermore, controllable spin-orbit interaction offers a way to achieve room temperature spin-charge conversion and generation of spin currents [93] for spintronics implementations.

However, spin-orbit coupling was often considered to be too small of an effect to contribute to the transport properties of the interface on a much bigger scale than quantum corrections. Contrary to this belief, Diez et al. [51] demonstrated that the semiclassical conductivity of spin-orbit coupled electrons scattered by extended impurities is surprisingly very sensitive to an in-plane magnetic field, that may explain the large drop of the in-plane magnetoresistance (up to 70% reduction at \(B = 12\) T) measured by the experiments. Furthermore, the semiclassical model provides a simple explanation for the striking similarity between gate-voltage– and temperature–dependence of the magnetoresistance.

Here we use the same semiclassical framework to investigate the dependence of the full resistivity tensor as a function of the magnitude and the in-plane orientation of the magnetic field, revealing the onset and peculiar evolution of a strongly anisotropic response. The large anisotropy survives within a range of chemical potentials such that multiple electronic subbands, with different dispersions and orbital polarizations, are populated at the same time. In this regime, the anisotropic magnetoresistance comes from a complex interplay of inter-band and intra-band scattering processes.

The structure of the chapter is as follows. In Sec. 2.2 we report and discuss the results of two magnetotransport experiments at \(\text{LaAlO}_3 / \text{SrTiO}_3\)
interfaces. In Sec. 2.3 we introduce the various ingredients of the theoretical model employed for transport calculations. In Sec. 2.4 we present the numerical results. In Sec. 2.5 we extensively discuss how our results arise from the interplay of spin-orbit coupling and magnetic field that dramatically affects the amplitudes of scattering between Bloch states. Sec. 2.6 contains a final summary and outlook. Details about the parameters of the model and additional results are provided in the Appendices.

2.2 Anisotropic planar magnetotransport: experimental signatures

To date there is a very broad collection of experimental studies [26, 36, 42, 49–52, 84–86, 90, 94] of the conducting (001) LAO / STO interface in the presence of an external magnetic field $B$. Here we restrict to electrical transport at low temperature (yet above the superconducting critical temperature $T_c \approx 300$ mK), and to magnetic field applied in the plane of the interface.

First striking observation is the abrupt change of the qualitative behavior of the measured resistance when the carrier density is tuned across the Lifshitz point in the band structure of the interface [36], by tuning the density of carriers via an applied gate voltage. Joshua et al. [50] reported the angular–dependence of the longitudinal ($\rho_{xx}$) and transverse ($\rho_{xy}$) resistivity measured at a Hall-bar device, by tuning the carrier density with a back-gate (back-gated), as a function of the planar angle between the current running between source and drain contacts and applied field. At low gate-voltage $\rho_{xx}$ depend very weakly on the orientation $\phi_B$ of the magnetic field relative to the direction of the current, and the maximum and minimum resistivity are measured along the crystalline axes. At high voltage the response of the system is extremely sensitive to the magnetic field: a large drop in $\rho_{xx}$ while increasing the field-strength occurs above a characteristic field $B_c$ of order of a few T. The latter is shown to have a dependence on the gate-voltage $V_G$, e.g. decreasing while increasing $V_G$ and diverging while approaching the Lifshitz point from above. Moreover the magnetoresistance is strongly anisotropic and its angular modulation is considered as the signature of a change of some symmetry of the system. Additional peaks and dips points appears at intermediate angles. The percentage of anisotropy measured at $B = 14$ T is about 20% of the average resistivity. Along with that, the authors report an abrupt increase of the transverse resistivity $\rho_{xy}$ by increasing the field. At a field larger than 10 T,
$\rho_{xy}$ becomes comparable to $\rho_{xx}$ and characterized by a striking step-like angular modulation.

The magnitude of $\rho_{xy}$ and its symmetry ($\rho_{xy} \approx \rho_{yx}$) rule out any relevant contributions of the orbital field due either to minimal misalignment between the direction of $B$ and the plane of the interface, or to the finite extension of the gas in the out-of-plane direction. The crystalline symmetry of the anisotropic response is revealed by the evolution of the direction of the principal axes of the resistivity tensor. While at low voltage (density) the principal axes follow the direction of $B$, at high voltage and high magnetic field the principal axes are pinned to diagonal directions ($45^\circ$, $135^\circ$, $225^\circ$, $315^\circ$): the directions where maximum and minimum resistivity are measured do not depend on the orientation of the magnetic field.

Similar behavior on different samples was previously reported by Ben Shalom et al. [85] who also investigated the temperature–dependence of the effect. Sharp minima (maxima) of the longitudinal resistivity are measured when the magnetic field is perpendicular (parallel) to the current. The magnitude of the high-field anisotropy is consistent with the finding of Joshua et al. [50] and is suppressed on the same temperature-scale which governs the magnetoresistance [51].

2.3 Electronic structure and the Boltzmann equation with correlated disorder

The low-energy electronic structure is obtained from the single-particle Hamiltonian introduced by Ruhman et al. [48]. In terms of creation (annihilation) operators $c_{k,l,\sigma}^\dagger$ ($c_{k,l,\sigma}$) of an electron with momentum $k$ in the $l = (d_{xy}, d_{xz}, d_{yz})$ orbital, the tight-binding Hamiltonian is

$$H = \sum_{k, l, l', \sigma, \sigma'} c_{k, l, \sigma}^\dagger H_{l, \sigma, l', \sigma'}(k) c_{k, l', \sigma'},$$

including the kinetic term $H_L$, the atomic spin-orbit coupling $H_{SO}$, the inversion-symmetry-breaking inter-orbital coupling $H_Z$ and the Zeeman coupling of the magnetic field with spin and angular orbital momentum (see Sec. 2.7 for the details).

The energy spectrum near the Lifshitz point is plotted in Fig. 2.1. At low density only $d_{xy}$ states are populated, with a tiny Rashba spin-splitting — proportional to $\alpha_R \sim \Delta_Z \Delta_{SO}/\Delta_E$ [95] ($\Delta_Z$ and $\Delta_{SO}$ are the
2.3 Electronic structure and the Boltzmann equation

![Dispersion and Equi-energy Contours](image)

**Figure 2.1:** (Top) Dispersion at \( k_y = 0 \) near the Lifshitz point, obtained by numerical diagonalization of the Hamiltonian 2.1. Different orbital polarizations are distinguished by different colors. (Bottom) Equi-energy contours at \( \epsilon - \mu = 0 \), showing the average spin and orbital angular momentum. Blue (yellow) arrows refer to the outermost (innermost) band of each pair. The complete set of parameters used for generating the plots are listed in the first row of Table 2.1 (Sec. 2.8).

Inversion-symmetry breaking and atomic spin-orbit parameter respectively, see Sec. 2.7). A change in the topology of the Fermi surface occurs at a threshold density, due to the onset of occupation of a new pair of bands.

The interplay of \( H_{SO} \) and \( H_Z \) produces strong orbital hybridization and spin-splitting for electronic states at points in the Brillouin zone where light and heavy bands would cross each other at \( H_{SO} = H_Z = 0 \). In the absence of magnetic field, analytical expressions for the effective Rashba-like coupling of the surface states of SrTiO\(_3\) and KTaO\(_3\) were derived by Kim et al. [96]. A similar derivation (valid near the \( \Gamma \)-point) was worked out by Zhou et al. [97]. Here we resort to numerical diagonalization of the Hamiltonian including the Zeeman coupling \( H_B = \mu_B (\mathbf{L} + g \mathbf{S}) \cdot \mathbf{B} / \hbar \) of the
magnetic field $B$ with the orbital ($L$) and spin ($S$) angular momentum. As shown in Fig. 2.1, at $T = 0$ the Fermi level is characterized by two small surfaces, elongated along the symmetry axes of the crystal, and two larger and less anisotropic ones. Importantly, the group velocity $v_{k,\nu} = \hbar^{-1} \frac{\partial \epsilon_{k,\nu}}{\partial k}$ is no longer parallel to the momentum for large sections of the Fermi surfaces.

We calculate the expectation-value of the spin and orbital angular momentum operators on the eigenstates. At $B = 0$, the $z$-component of both is quenched to zero because of time-reversal and $\pi$-rotation symmetry around the $z$-axis and will stay zero as long as the magnetic field has no component in the out-of-plane direction. Following the evolution of the expectation-value of the spin on the large Fermi surfaces in the top-right quadrant of the Brillouin zone ($\vartheta < 90^\circ$), it is found to be parallel to the $y$-axis at small $\vartheta$ (small $k_y$), it suddenly undergoes a $90^\circ$-rotation in the vicinity of $\vartheta = 45^\circ$ and finally aligns to the $x$-axis at $\vartheta > 45^\circ$. The magnitude of the average orbital angular momentum is peaked near the hybridization gaps while it is very small on the remaining sectors of the Fermi surfaces. Electronic spectrum and the spin-orbital structure at the Fermi level are consistent with the data reported by King et al. [98] for the surface states of SrTiO$_3$.

The eigenstates $|\psi_{k,\nu}\rangle = |u_{k,\nu}\rangle e^{ik \cdot r}$ and the eigenvalues $\epsilon_{k,\nu}$ of the Hamiltonian 2.1 enter the Boltzmann transport equation

$$-e(v_{k,\nu} \cdot E) \frac{\partial f_0}{\partial \epsilon_{k,\nu}} = \sum_{k',\nu'} (g_{k,\nu} - g_{k',\nu'}) q_{k\nu,k'\nu'} \delta(\epsilon_{k,\nu} - \epsilon_{k',\nu'}),$$

(2.2)

that returns returning the out-of-equilibrium shift $g_{k,\nu}$ in the electron distribution function due to an accelerating electric field $E$ and scattering by impurity centres. $f_0(\epsilon)$ is the equilibrium Fermi-Dirac distribution function and $v_{k,\nu} = \hbar^{-1} \frac{\partial \epsilon_{k,\nu}}{\partial k}$. Spatial correlations between different impurities can be introduced via a Gaussian potential

$$U(r) = \sum_i U_i e^{-|r-r_i|^2/\xi^2}.$$  

(2.3)

where the amplitudes $U_i$ of the individual scatterers are randomly distributed with uniform probability in the symmetric range $[-\delta/2, \delta/2]$ and $\xi$ is the characteristic decay-length of the two-point correlator (that is Gaussian as well).

At leading order in the Born approximation and averaging over the ensemble of impurity configurations, the amplitude of elastic scattering
2.4 Numerical results

from the initial state $|u_{k\nu}\rangle$ to the final state $|u_{k'\nu'}\rangle$ is

$$q_{k\nu,k'\nu'} = \frac{2}{3\pi^3} \hbar^{-1} \delta^2 \xi^4 n_{\text{imp}} e^{-\xi^2 |k-k'|^2/2} |\langle u_{k\nu} | u_{k'\nu'} \rangle|^2,$$  \hspace{1cm} (2.4)

$n_{\text{imp}}$ being the density of impurities.

An alternative model was considered by Fu et al. [99] who calculated the density-dependence of the resistivity in multi-subband accumulation layers (heterojunctions of polar and non-polar perovskites such as LAO and STO) where electrons are scattered by the potential generated by surface roughness. In their model, spatial disorder-correlations decay exponentially. In momentum-space, the elastic scattering amplitude

$$q_{k\nu,k'\nu'} = \frac{2\pi^2 \delta^2 \xi^2}{\hbar} n_{\text{imp}} (1 + \xi^2 |k-k'|^2)^{-3/2} |\langle u_{k\nu} | u_{k'\nu'} \rangle|^2$$  \hspace{1cm} (2.5)

decays algebraically as a function of the momentum transferred to the impurity ($q_{k\nu,k'\nu'} \propto |k-k'|^{-3}$ at large $|k-k'|$). The scattering with large momentum-transfer (and hence backscattering) is stronger for this model than for the Gaussian model of Eq. (2.4).

Here we only consider scalar impurities, described by single-impurity-potential operators that are diagonal in the basis of the unperturbed Hamiltonian. The scattering processes can occur from a band to itself ("intra-band"), or to a different one ("inter-band").

We present results of magnetotransport calculations for two models of disorder — Gaussian-correlated impurities and surface-roughness — that show a similar behavior of the fixed-density magnetoresistance, albeit the density-dependence of bare resistance may be substantially different in the two cases [99].

2.4 Numerical results

At linear order in the electric field $\mathbf{E}$, the out-of-equilibrium distribution $g_{k\nu}$ is in terms of the band- and momentum-dependent vector mean-free-path $\Lambda_{k\nu}$ [100] is

$$g_{k\nu} = -e(\partial f_0/\partial \epsilon_{k\nu}) \mathbf{E} \cdot \mathbf{\Lambda}_{k\nu}.$$  \hspace{1cm} (2.6)

Eigenvalues $\epsilon_{k\nu}$ and eigenvectors $u_{k\nu}$ of the Hamiltonian in Eq.(2.1) are calculated numerically. for each value of the in-plane magnetic field ($B \cos \phi_B, B \sin \phi_B$), where $\phi_B$ is the angle measured counterclockwise from the $x$-axis. The electron density is kept constant at any $B$. as a consequence, therefore the chemical potential $\mu(B, \phi_B) \equiv \mu(B)$ is determined

29
self-consistently according to

\[ n_e = \int_{\epsilon_0}^{\infty} d\epsilon f_0(\epsilon, \mu(B), T) N(\epsilon), \quad (2.7) \]

where \( N(\epsilon) \) is the density of states at energy \( \epsilon \) and \( \epsilon_0 \) the energy of the bottom of the lowest conduction band.

The conductivity tensor \( \sigma \) follows from the distribution function as

\[ (\sigma)_{ij} = e \sum_{k,\nu} (v_{k,\nu})_i \frac{\partial g_{k,\nu}}{\partial E_j}. \quad (2.8) \]

By matrix-inversion of \( \sigma \) we finally extract the longitudinal resistivity and the transverse resistivity, as

\[ \rho_{xx} = \frac{\sigma_{yy}}{\sigma_{xx} \sigma_{yy} - \sigma_{xy}^2}, \quad \rho_{xy} = -\frac{\sigma_{xy}}{\sigma_{xx} \sigma_{yy} - \sigma_{xy}^2}. \quad (2.9) \]

In this section we show the results of calculations performed at a temperature \( T = 1 \) K and a carrier-density \( n = 2.2 \times 10^{13} \) cm\(^{-2} \), corresponding to a chemical potential crossing the second pair of bands. Two bands remain a few meV \( (\approx \Delta_{SO}/2) \) higher than \( \mu \) and do not play any role here since we only consider elastic scattering. (The spin-orbit gap between \( d_{xz} \) and \( d_{yz} \) states is much larger than the thermal broadening of the Fermi-Dirac distribution.)

In Fig. 2.2 the magnetoresistance \( \rho_{xx}(B)/\rho_{xx}(0) - 1 \) and the transverse resistivity \( \rho_{xy} \) are plotted as a function of the angle \( \phi_B \), for values of \( B \) between 2 and 20T. The transverse resistivity has been rescaled by its maximum value at 10T — obtained around \( \phi_B = 45^\circ \) — in order to get a quantity that (as the magnetoresistance) is independent of the parameters \( n_{imp} \) and \( \delta \). In the range between 4 and 10 T (at lower fields the effects are moderate) the angular modulation of the magnetoresistance has cusp-like dips at \( \phi_B = 90^\circ, 270^\circ \) (magnetic field perpendicular to the current) and rounded maxima at \( \phi_B = 0^\circ, 180^\circ \) (magnetic field aligned to the current). The magnitude of the negative magnetoresistance and the anisotropy progressively increase with the field-strength. The transverse resistivity has a sinusoidal modulation with maxima and minima shifted by 45° with respect to the magnetoresistance extrema. However \( \rho_{xy} \) is two orders of magnitude smaller than \( \rho_{xx} \). Above 10 T, the angular magnetoresistance develops additional maxima and minima near diagonal orientations \( (\phi_B = 45^\circ, 135^\circ, 225^\circ, 315^\circ) \) that unlike the main extremal points — fixed at multiples of 90° — do not only move up and down.
2.4 Numerical results

Figure 2.2: (Top) Magnetoresistance \( \rho_{xx}(B)/\rho_{xx}(0) - 1 \) and (bottom) transverse resistivity \( \rho_{xy} \) (rescaled by the maximum \( \rho_{xy} \) at \( B = 10 \text{T} \)), as a function of the angle between the direction of the magnetic field and the \( x \)-axis, at different values of the field-strength. The left panel is for calculations with scattering by Gaussian-correlated impurities, with amplitudes from Eq. (2.4). The right panel is for calculations with scattering by surface-roughness disorder, with amplitudes from Eq. (2.5). The temperature is \( T = 1 \text{K} \) and the density \( n = 2.2 \times 10^{13} \text{cm}^{-2} \). Other parameters from the first row of Table 2.1 (Sec. 2.8).

but also shift in angular position as the field is progressively increased. In the same field-range where these additional features characterize the magnetoresistance, \( \rho_{xy} \) increases by (more than) one order of magnitude. Another striking feature is the change in the angular modulation of the transverse resistivity that substantially deviates from the sinusoidal low-field behaviour. Other parameters are considered in Sec. 2.8.

The \( B \)-dependence of the magnetoresistance at different angles \( \phi_B \) is shown in Fig. 2.3. Amplitude, shape and the field-scale of the magnetoresistance, all change with \( \phi_B \). Moving from a configuration with magnetic field parallel to the direction of the current (\( \phi_B = 0^\circ \)) towards the opposite configuration (\( \phi_B = 90^\circ \)), the magnitude of the magnetoresistance grows by a factor \( \sim 3 \) at 20 T. Moreover, the field-scale where the slope of the
magnetoresistance becomes negative – and large in magnitude – decreases by moving the field away from the direction of the current. The results are consistent with previous calculations [51] of the magnetoresistance at \( \phi_B = 90^\circ \), albeit here calculated in a different spin-orbit–coupling regime (see Sec. 2.8). The angular-maximum of the transverse resistivity \( \rho_{xy} \) exhibits a strong enhancement around starting at \( \sim 10 \text{T} \) for the Gaussian model (slightly higher field for the exponential model).

The slope of \( \rho_{xy}(B) \) softens at the very high fields, where the magnetoresistance at \( \phi_B = 45^\circ \) shows the onset of saturation in the case of Gaussian disorder-potential. For the other model, instead, the curvature of the magnetoresistance at \( \phi_B = 45^\circ \) is still negative at \( B = 20 \text{T} \) (no saturation in this field-range) that also produces a non-saturating \( \rho_{xy} \).

### 2.5 Discussion

At \( T = 0 \) only electrons at the Fermi level contribute to the conductivity of a metal. In favour of a clearer discussion, hereafter we neglect the effects of a finite low temperature — these are crucial quantitatively, but do not alter the underlying mechanism.

At densities much lower than the threshold density of the Lifshitz transition \( (n_e \ll n_L) \), the chemical potential \( \mu(B) \) — determined at any \( B \) self-consistently according to Eq. (2.7) — lies deep into the \( d_{xy} \) bands, that have a tiny \( k \)-linear Rashba splitting [95]. In this regime, the anisotropy is
2.5 Discussion

extremely weak (less than 1%) (see Fig. 2.7 in Sec.2.8). A previous work shows that even the inclusion of spin-selective scatterering does not give any sizable anisotropy [101].

At densities slightly larger than $n_L$, instead, the chemical potential crosses the hybridization gaps where the spin-splitting is about ten times larger than at low density. We have not considered densities right at the Lifshitz transition to avoid artifacts in the numerics due to the sudden appearance of band-edges with almost-zero Fermi momentum.

For the scattering models of Eq. (2.4) and Eq. (2.5), in the outermost bands — characterized by large Fermi surfaces and high band velocities — the backscattering is suppressed for correlation lengths much larger than the inverse of the average Fermi momentum. Hence, relaxation via intra-band scattering takes place on a slow time-scale (that includes many low-angle scattering events), while the most effective mechanism of velocity relaxation is provided by forward-scattering processes to the inner bands. Indeed, the inner bands have low mobilities, due to the small velocities and large intra-band scattering rates.

At $B = 0$ the spin-ordering near the hybridization gaps in the top-right quadrant of the Brillouin zone is $|\downarrow\rangle|\uparrow\rangle|\uparrow\rangle|\downarrow\rangle$ (see Fig. 2.1b). At some non-universal value of $B$ (dependent on the specifics of the band structure), the ordering is reversed for the inner bands (not shown in the figure). This results in reduction of the scattering rates between pairs of states $(k, \nu)$ and $(k', \nu')$ that have minimal inter-band distances $|k - k'|$ and parallel spins at $B = 0$. The field-suppression of inter-band scattering leads to enhanced (reduced) longitudinal conductivity (resistivity) with increasing magnetic field. The enhancement is particularly large at orientations $\phi_B = 90^\circ, 270^\circ$, where the magnetic field is aligned to the spin-orbit field acting on states with the highest velocity $v_{k,\nu}$ in the direction of the electric field.

The qualitative behavior changes for $B > 10$ T, where the intra-band scattering starts giving a non-negligible contribution. In Fig. 2.4 the calculated vectors mean-free-path $\Lambda_{k,\nu}$ are plotted on top of the equi-energy contours at the Fermi level, for different magnetic-field configurations. At $\phi_B = 45^\circ$ (c–d), the magnetic field is far from the crystalline axis. The outermost contours (almost) cross each other at a polar coordinate $\vartheta = \bar{\vartheta} \approx 10^\circ$, but not at the complementary angle $(90^\circ - \bar{\vartheta})$ (top-right quadrant). As a consequence, the rates of scattering between $d_{xy}$-polarized (red) states — of polar coordinate $\bar{\vartheta} < \vartheta < 90^\circ - \bar{\vartheta}$ — and hybrid $d_{xy}/d_{xz}$ (purple) states at $\vartheta \approx \bar{\vartheta}$ are enhanced by the field, as opposed to the complementary-scattering rates.

To better illustrate the consequences of this, we formally express the
solution of the Boltzmann equation (2.2) in the recursive form

\[ \Lambda_{k,\nu} = v_{k,\nu} \tau_{k,\nu} + \sum_{k' \neq k} q_{k,\nu, k',\nu'} \left\{ v_{k',\nu'} \tau_{k',\nu'} + \sum_{k'' \neq k', k'} q_{k',\nu', k'',\nu''} \left( v_{k'',\nu''} \tau_{k'',\nu''} + \cdots \right) \right\}, \]  

(2.10)

where \( \tau_{k,\nu} \) is the bare band- and momentum-dependent relaxation-time

\[ \tau_{k,\nu} = \sum_{k',\nu'} q_{k,\nu, k',\nu'}. \]  

(2.11)

The low-angle scattering is strongly anisotropic, thereby the scattering-in corrections to the vector mean-free-path \( \Lambda_{k,\nu}^{\text{RTA}} = \tau_{k,\nu} v_{k,\nu} \) — calculated in relaxation-time approximation [102, 103] — substantially affect magnitude and direction of the vector mean-free-path, that gets tilted (away from the direction of the velocity \( v_{k,\nu} \)) towards the direction of enhanced scattering (\( \vec{\theta} \)). The anisotropy of the scattering effectively acts as a Lorentz force, driving a shift of the electron distribution around the equi-energy contours [104, 105]. However, unlike the actual Lorentz force, magnitude and direction of this “effective Lorentz force” at a point \((k, \nu)\) change non monotonically as a function of the magnetic-field parameters \( B \) and \( \phi_B \), and so do the intra-band scattering rates. The direction of the tilting of the vector mean-free-path \( \Lambda_{k,\nu} \) may then undergo multiple reversals when the magnetic field changes in magnitude and/or direction, thereby the out-of-equilibrium distribution

\[ g_{k,\nu} \propto \Lambda_{k,\nu} \cdot E \]  

(2.12)

can increase or decrease, depending on whether the direction of the tilting “tends” to the direction of the electric field or not. The appearance of secondary maxima and minima (whose positions also change with \( B \)) of the magnetoresistance vs. field curves, when the field is along intermediate directions away from the crystalline axes, is explained by the field-dependence of the effective Lorentz force.

Unlike the longitudinal magnetoresistance, the transverse resistivity \( \rho_{xy} \) is entirely dominated by the intra-band scattering, that is the reason why it is substantially zero for \( B \lessgtr 10 \text{T} \). We need to look at the total contribution to the conductivity carried by states with opposite velocities
2.5 Discussion

![Figure 2.4](image)

**Figure 2.4:** Fermi surfaces at $n = 2.2 \times 10^{13} \text{cm}^{-2}$ for different configurations of the in-plane magnetic field: (a) $B = 0 \text{T}$, (b) $B = 20 \text{T}$ $\phi_B = 90^\circ$, (c) $B = 10 \text{T}$ $\phi_B = 45^\circ$, (d) $B = 20 \text{T}$ $\phi_B = 45^\circ$. Magnitude and direction of the vector mean-free-path $\Lambda_k$ as a function of the momentum $k$ on the outermost bands (which support all of the total conductivity at any fields) are represented by arrows - colors distinguish the two bands of each pair. The longitudinal conductivity $\sigma_{xx}$ is proportional to the average $x$-component of the vector mean-free-path. (At $\phi_B = 0$, $90^\circ$, $\rho_{xx} = \sigma_{xx}^{-1}$.) The modulation of the vector mean-free-path in (c) is mirror-symmetric with respect to the crystalline axes; therefore $\sigma_{xy}(\rho_{xy}) \approx 0$ because states with opposite velocities compensate each other with equal weights $\Lambda^x$. Instead in (d) the texture of the vector mean-free-path is manifestly asymmetric, producing sizable $\sigma_{xy}$. 

35
in the direction perpendicular to the electric field and understand why an imbalance between their occupations is generated by the magnetic field. For the states in the bottom-right quadrant \((270^\circ < \vartheta < 360^\circ)\), the scattering-in rates are large and isotropic, thereby they only affect the magnitude — but not the direction — of the vector mean-free-path. Hence \(\Lambda_{k,\nu} \propto v_{k,\nu}\) still holds, although the proportionality coefficient deviates from the bare relaxation-time \(\tau_{k,\nu}\). Similarly, states in the top-left quadrant of the Brillouin zone have \(\Lambda_{k,\nu} \propto v_{k,\nu}\). However the latter receive smaller scattering-in corrections because the magnetic field does not reduce — but rather enhances — the spin-orbital splitting at any point in the quadrant. This imbalance is large enough to produce an unexpectedly-large \(\rho_{xy}\) \((\rho_{xy}/\rho_{xx} \approx 0.1\) at \(B = 20\text{T})\) even in the absence of orbital effects of the magnetic field.

Finally, the angular modulation of \(\rho_{xy}\) sharply ramp up when the angle \(\phi_B\) takes a value such that at isolated points in the Brillouin zone the spin-orbital splitting is totally suppressed by the Zeeman field. Once this occurs, the low-angle scattering abruptly develops a preferential direction, and then remains stable until the field is rotated far enough to let the spin-orbital splitting open again. This results in a flattening of the peaks of \(\rho_{xy}\) more or less pronounced in all the plots shown in this chapter.

### 2.6 Conclusions

In this work, we have investigated magnetotransport at the LaAlO\(_3\)/SrTiO\(_3\) interface with a simple theoretical model based on semiclassical Boltzmann transport. In particular, we have studied the dependence of the resistivity tensor on the magnitude and orientation of an in-plane magnetic field, leaving out the investigation of the effects of an orbital field.

Many-body effects, e.g. electron-electron \([106, 107]\) and magnetic interactions \([48, 50]\), are neglected. Spin-orbit coupling effects on the low-energy states of the conduction band are included by means of an effective tight-binding model including three atomic orbitals. The Boltzmann equation (2.2) for electrons scattered by correlated impurities — with correlations decaying on a characteristic length scale \(\xi\) — is solved numerically as a function of the external field. Our main finding is a crossover from the low-field regime of weak anisotropy to the high-field regime of strong anisotropy which results from important changes in the electronic structure at the Fermi level when the carrier-density is tuned above the Lifshitz point \([48]\). However, we remark that is not simply the onset of the occupation of anisotropic bands to determine a change of
2.7 Appendix A. Single-particle Hamiltonian

To model the conduction bands at the interface we use a single-electron Hamiltonian [48] where the electronic states are derived from the $t_{2g}$ ($d_{xy}$, $d_{xz}$ and $d_{yz}$) orbitals of Ti-atoms. Accounting for a total number of six degrees of freedom (three orbitals times two spin components), the translational invariant Hamiltonian in momentum space has a $6 \times 6$ matrix-representation that is the sum of the four terms in Eq. (2.1). The kinetic Hamiltonian

$$H_L = \left( \begin{array}{ccc} \epsilon_{xy}(k) - \Delta_E & 0 & 0 \\ 0 & \epsilon_{xz}(k) & \delta(k) \\ 0 & \delta(k) & \epsilon_{yz}(k) \end{array} \right) \otimes \hat{\sigma}_0, \quad (2.13)$$

$$\epsilon_{xy}(k) = 2t_l(2 - \cos k_x - \cos k_y),$$
$$\epsilon_{xz}(k) = 2t_l(1 - \cos k_x) + 2t_h(1 - \cos k_y),$$
$$\epsilon_{yz}(k) = 2t_h(1 - \cos k_x) + 2t_l(1 - \cos k_y),$$
$$\delta(k) = 2t_d \sin k_x \sin k_y.$$ (2.14)

describes electrons hopping between Ti-orbitals on adjacent sites in the interfacial ($xy$) plane. $d_{xy}$ orbitals have all the lobes lying on the $xy$-plane, $x$- and $y$- hopping amplitudes are equivalently described by a single light matrix elements $t_l$. Instead $d_{xz}$ and $d_{yz}$ orbitals have both lobes in-plane and in the direction normal to the interface, giving rise to one light and one heavy ($t_h < t_l$) matrix element, respectively. $\Delta_E$ is the gain in the on-site energy of $d_{xy}$ states confined at the interface compared to the on-site energy of $d_{xz}$/$d_{yz}$ states. Inter-orbital matrix elements $\propto \sin k_x \sin k_y$
account for $d_{xz}/d_{yz}$ hybridization with a strength $t_d \approx t_h$ (however, this term does not affect at all the results of our calculations).

At the interface the confining electric field along the $z$-direction breaks the inversion-symmetry and activates transitions from $d_{xy}$ orbitals – which are even under mirror symmetry – to $d_{xz}$ and $d_{yz}$ orbitals – odd under mirror symmetry – on adjacent metal sites. The inversion-breaking term has the form

$$H_Z = \Delta_Z \begin{pmatrix} 0 & i \sin k_y & i \sin k_x \\ -i \sin k_y & 0 & 0 \\ -i \sin k_x & 0 & 0 \end{pmatrix} \otimes \hat{\sigma}_0. \quad (2.15)$$

Atomic spin-orbit coupling is the same as for the bulk STO system, that is

$$H_{SO} = \frac{\Delta_{SO}}{2} \sum_{i=x,y,z} \sigma_i \otimes L_i = \frac{\Delta_{SO}}{2} \begin{pmatrix} 0 & i\hat{\sigma}_x & -i\hat{\sigma}_y \\ -i\hat{\sigma}_x & 0 & i\hat{\sigma}_z \\ i\hat{\sigma}_y & -i\hat{\sigma}_z & 0 \end{pmatrix}, \quad (2.16)$$

with

$$L_x = \hbar \begin{pmatrix} 0 & i & 0 \\ -i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad L_y = \hbar \begin{pmatrix} 0 & 0 & -i \\ 0 & 0 & i \\ -i & i & 0 \end{pmatrix}, \quad L_z = \hbar \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & i \\ 0 & -i & 0 \end{pmatrix} \quad (2.17)$$

the representations of the components of the orbital angular momentum. Lastly, the Zeeman Hamiltonian $H_B = \mu_B (L + gS) \cdot B / \hbar$ is

$$H_B = \mu_B \begin{pmatrix} g(B_x \hat{\sigma}_x + B_y \hat{\sigma}_y)/2 & iB_x \sigma_0 & -iB_y \sigma_0 \\ -iB_x \sigma_0 & g(B_x \hat{\sigma}_x + B_y \hat{\sigma}_y)/2 & 0 \\ iB_y \sigma_0 & 0 & g(B_x \hat{\sigma}_x + B_y \hat{\sigma}_y)/2 \end{pmatrix}, \quad (2.18)$$

with $B_x = |B| \cos \phi_B$, $B_y = |B| \sin \phi_B$ and $S = \hbar \hat{\sigma} / 2$.

### 2.8 Appendix B. Dependence of the anisotropy on the parameters of the model

The parameters which define the model of the interface are taken within the ranges that are set by theoretical and experimental results in literature, e.g. first-principles calculations, ARPES measurements on the cleaved surface of strontium titanate [98, 108, 109] and, more recently, soft-X-ray ARPES on the LAO / STO interface [110]. Further estimates from transport measurements [35, 84, 94, 111] give more informations at least about the
order of magnitude of the energy scales in the system. In Table 2.1 we list and discuss the choice of the parameters used for our calculations and in addition we show results for different values of parameters. The comparison with the results in the main text highlight the robustness of the most remarkable features of the data that we have previously highlighted. (The calculations here are for Gaussian-correlated impurities.)

<table>
<thead>
<tr>
<th>Fig.</th>
<th>(t_l)</th>
<th>(t_h)</th>
<th>(\Delta E)</th>
<th>(\Delta_{SO})</th>
<th>(\Delta_Z)</th>
<th>(g)</th>
<th>(\xi)</th>
</tr>
</thead>
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<td>2.2, 2.3, 2.7</td>
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<td>12.5</td>
<td>65</td>
<td>7</td>
<td>2.5</td>
<td>5</td>
<td>5</td>
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<tr>
<td>2.5</td>
<td>400</td>
<td>12.5</td>
<td>65</td>
<td>9</td>
<td>4</td>
<td>−3.4</td>
<td>5</td>
</tr>
<tr>
<td>2.6</td>
<td>400</td>
<td>12.5</td>
<td>65</td>
<td>7</td>
<td>2.5</td>
<td>5</td>
<td>4, 8</td>
</tr>
</tbody>
</table>

Table 2.1: Sets of parameters used for the magnetotransport calculations in the chapter, with reference to the figures.

Hopping elements \(t_l\), \(t_h\), confinement energy \(\Delta E\), atomic-spin orbit strength \(\Delta_{SO}\) and inversion-asymmetry parameter \(\Delta_Z\) are measured in meV; the \(g\)-factor is dimensionless and the disorder correlation-length \(\xi\) is measured in units of the lattice constant \(a\). The values of the light and heavy mass corresponding to the hopping parameters \(t_l\) and \(t_h\) are 0.6 \(m_e\) and 19 \(m_e\) respectively (\(m_e\) is the bare electron mass).

The value of \(\Delta_{SO}\) from ab-initio calculations [112] or transport experiments [35, 84] is estimated in a wide range 10 ÷ 25meV. (In a seminal work on Raman scattering for the bulk STO system Uwe et al. [113] extracted the value 18meV). Here we consider the values \(\Delta_{SO} = 7\) meV and \(\Delta_{SO} = 9\) meV (so just below the lower limit of the estimated range) and produce qualitatively similar results for the anisotropy, while at the same time changing also \(g\) and \(\Delta_Z\). In principle one could take larger values of \(\Delta_{SO}\) and slightly different hopping elements and still remain in a regime where our results still hold. Moreover, we point out that the strong anisotropy of the spin-orbit field around the Fermi surfaces [98] – with a large enhancement of the effective orbital angular momentum near hybridization gaps – so far has not been considered in fitting transport measurements, that might return overestimated values of \(\Delta_{SO}\).

Outcomes of Boltzmann calculations [51] were found in good agreement with the experimentally measured magnetoresistance at \(\phi_B = 90^\circ\) (no
transverse current, hence $\sigma_{xy} = 0$) in the regime of strong inversion-symmetry-breaking $\Delta_Z > \Delta_{SO}$. Here we obtain similar magnetoresistance – and comparable field-dependence – in the different (and maybe more realistic) regime $\Delta_Z < \Delta_{SO}$. We can understand this similarity observed in two completely different regimes by realizing that the reversal of the spin-ordering on neighbouring Fermi surfaces induced by the magnetic field, which reduces the overall forward scattering and hence lowers the resistance, occurs in both cases regardless of the relative orientation of orbital and spin angular momenta (which is different in the two regimes). For $\Delta_Z$ we consider values up to 5 meV, that is the upper bound estimated by Ruhman et al. [48].

It is known that the $g$-factor for electrons confined in quantum wells, like InSb and GaAs [114] can substantially differ from the conventional value $g = 2$. In Sec. 2.4 we show results for $g = 5$, one of the two possible outcomes (the other one is $g = -3.4$) of a fit to Shubnikov-de Haas oscillations at low temperature [94]. (Note that changing the $g$-factor is not simply equivalent to rescale the magnetic field: magnetic field also couples to the orbital angular momentum and the relative strength

Figure 2.5: Magnetoresistance and transverse resistivity for a negative $g$-factor (parameters from the second row of Table 2.1).
2.8 Appendix B. Dependence of the anisotropy on the parameters

Figure 2.6: Magnetoresistance and transverse resistivity for different values of the correlation-length $\xi$ (parameters from the third row of Table 2.1).

$(\mathbf{\mu} \cdot \mathbf{B})/(\mathbf{L} \cdot \mathbf{B})$ is dependent on $g$. Yet the phenomenology of the anisotropy which we extensively discussed in Sec. 2.5 is recovered at negative $g = -3.4$ (Fig. 2.5).

Variations in the correlation-length $\xi$ are also considered. While there is no simple way to extract informations from experiments, it is reasonable to limit $\xi$ within a range of one order of magnitude. Indeed, a too large $\xi (> 10 a_0$ with $a_0 = 0.4\text{nm}$ the lattice constant) would require to treat the impurities as a disordered medium rather than independent scatterers. Calculations in the main text refer to $\xi = 5 a_0$. In Fig. 2.6, results for $\xi = 4, 6, 8$ are shown. Qualitatively the results are very similar if $\xi |\Delta k^{bs}| > 1$ where $|\Delta k^{bs}| \sim 2k_F^{out}$ is the momentum-transfer for backscattering in the large outer band (approximately equal to twice the average Fermi momentum) and at the same time not larger than $10 – 15 a_0$ – with $a_0 = 0.4\text{nm}$ the lattice constant – whereby also the zero-field inter-band scattering is highly reduced. This upper limit is also consistent with the assumption of scattering by individual impurities (rather than by a disordered medium that is a more suitable description for very large $\xi$).

Finally, we shortly comment on the density– vs. field–dependence of the resistivities. Universal scaling of the magnetoresistance curves as a function of carrier-density, after the magnetic field is rescaled by a density–dependent characteristic value, appears to be a general feature of the experimental data [50, 51]. This is not recovered by the Boltzmann
model (even within this different spin-orbit regime) pointing to a physical mechanism that might be unrelated to spin-orbit coupling.

In Fig. 2.7 we show results of calculations at two different densities, \( n = 1.5 \cdot 10^{13}\text{cm}^{-2} \) (below the Lifshitz point) and \( n = 2.1 \cdot 10^{13}\text{cm}^{-2} \) (above the Lifshitz point). The total absence of magnetoresistance at the lowest density (left panel) simply comes from the absence of inter-band scattering (since only the lowest \( d_{xy} \) states are filled). At higher density (right panel) the large-field magnetoresistance is characterized by multiple maxima and minima as in Fig. 2.2, but there is larger discrepancy between the magnetoresistance calculated at \( \phi_B = 0 \) and the one at \( \phi_B = 90 \). This gap is progressively reduced as the chemical potential tends to the middle of the spin-orbit gap at the \( \Gamma \)-point.