

# Disentangling surface and bulk transport in topological insulator $p$ - $n$ junctions

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By combining  $n$ -type  $\text{Bi}_2\text{Te}_3$  and  $p$ -type  $\text{Sb}_2\text{Te}_3$  topological insulators, vertically stacked  $p$ - $n$  junctions can be formed, allowing to position the Fermi level into the bulk band gap and also tune between  $n$ - and  $p$ -type surface carriers. Here we use low-temperature magnetotransport measurements to probe the surface and bulk transport modes in a range of vertical  $\text{Bi}_2\text{Te}_3/\text{Sb}_2\text{Te}_3$  heterostructures with varying relative thicknesses of the top and bottom layers. With increasing thickness of the  $\text{Sb}_2\text{Te}_3$  layer we observe a change from  $n$ - to  $p$ -type behavior via a specific thickness where the Hall signal is immeasurable. Assuming that the bulk and surface states contribute in parallel, we can calculate and reproduce the dependence of the Hall and longitudinal components of resistivity on the film thickness. This highlights the role played by the bulk conduction channels which, importantly, cannot be probed using surface sensitive spectroscopic techniques. Our calculations are then buttressed by a semi-classical Boltzmann transport theory which rigorously shows the vanishing of the Hall signal. Our results provide crucial experimental and theoretical insights into the relative roles of the surface and bulk in the vertical topological  $p$ - $n$  junctions.

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## I. INTRODUCTION

Topological insulators (TIs) are bulk insulators with exotic ‘topological surface states’<sup>1</sup> (TSS) which are robust to backscattering from non-magnetic impurities, exhibit spin-momentum locking<sup>2</sup> and have a Dirac-like dispersion<sup>3–5</sup>. These unique characteristics present several opportunities for applications in spintronics, thermoelectricity, and quantum computation. However, a major drawback of ‘early generation’ TIs such as  $\text{Bi}_{1-x}\text{Sb}_x$ <sup>5</sup> and  $\text{Bi}_2\text{Se}_3$ <sup>2,3</sup> is that the Fermi level  $E_F$  intersects the conduction/valence bands, thus giving rise to finite conductivity in the bulk. This non-topological conduction channel conducts in parallel to the TSS and in turn subverts the overall topological nature. Thus, in order to create bona fide TIs, the Fermi level  $E_F$  needs to be tuned within the bulk bandgap, and this has previously been achieved by means of electrical gating<sup>6–9</sup>, doping<sup>4,10?, 11</sup>, or, as recently reported, by creating  $p$ - $n$  junctions from two different TI films<sup>13,14</sup>.

In Ref. 14 a ‘vertical topological  $p$ - $n$  junction’ was realized by growing an  $n$ -type  $\text{Bi}_2\text{Te}_3$  layer capped by a layer of  $p$ -type  $\text{Sb}_2\text{Te}_3$ , and it was shown that varying the relative layer thicknesses serves to tune  $E_F$  without the use of an external field. Importantly, such bilayer systems are expected to be significantly less disordered than doped materials such as  $(\text{Bi}_{1-x}\text{Sb}_x)_2\text{Te}_3$  in which inhomogeneity of the dopants is a constant problem<sup>15?</sup>. Furthermore, and in sharp contrast to doped TIs, the intrinsic  $p$  and  $n$  character of the individual layers presents re-

markable opportunities towards the observation of novel physics including Klein tunneling<sup>16,17</sup>, spin interference effects at the  $p$ - $n$  interface<sup>18</sup>, and topological exciton condensates<sup>19</sup>. However, currently there exists little understanding of the bulk conduction in such topological  $p$ - $n$  junctions, primarily because ARPES used in Ref. 14 is a surface-sensitive method. This is especially noteworthy in light of the fact that the band structure varies along the depth of the TI  $p$ - $n$  junction slab, in sharp contrast to the essentially constant band gap within the bulk of  $(\text{Bi}_{1-x}\text{Sb}_x)_2\text{Te}_3$ -type compounds. Understanding and minimizing the bulk conduction channels in TI  $p$ - $n$  junctions is crucial in order to realize their technological potential as well as to gain access to the exotic physics they can host.

## II. EXPERIMENT

$\text{Bi}_2\text{Te}_3/\text{Sb}_2\text{Te}_3$ -bilayers (BST) were grown on phosphorous doped Si substrates using molecular beam epitaxy (MBE). Details of the MBE sample preparation can be found in Ref. 14. In all the samples, the bottom  $\text{Bi}_2\text{Te}_3$ -layer had thickness  $t_{\text{BiTe}} = 6$  nm while the top  $\text{Sb}_2\text{Te}_3$ -layers had thicknesses  $t_{\text{SbTe}} = 6.6$  nm (BST6), 7.5 nm (BST7), 15 nm (BST15), and 25 nm (BST25), respectively. The layers were patterned into Hall bars of width  $W = 200$   $\mu\text{m}$  and length  $L = 1000$   $\mu\text{m}$  using photoresist as a mask for ion milling, and Ti/Au contact pads were deposited for electrical contact. Low- $T$  electrical

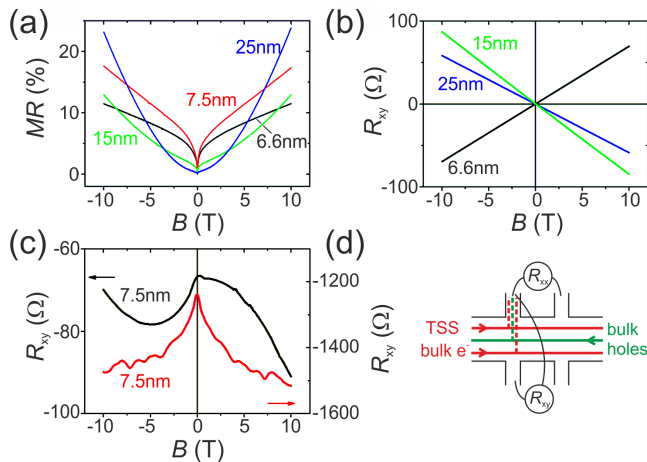


FIG. 1. (a) MR and (b+c)  $R_{xy}$  as a function of  $B$  for different  $t_{\text{Sb}_2\text{Te}_3}$ . All curves are measured at 280 mK. The high field MR is linear for thin samples and changes to parabolic for thicker samples. Cusp-like deviations at low fields are due to WAL corrections. The sign change of the slope in (b) indicates transport by electrons for BST6 and by holes for BST15 and BST25. No Hall slope is visible in (c) for 2 different pairs of contacts of BST7. (d) The schematic shows the charge transport channels in a longitudinal and transverse measurement setup. Trajectories of TSS and bulk electrons are shown in red and of bulk holes in green.

69 measurements were carried out using lock-in techniques  
70 in a He-3 cryostat with a base temperature of 280 mK and  
71 a 10 T superconducting magnet. Both longitudinal ( $R_{xx}$ )  
72 and transverse ( $R_{xy}$ ) components of resistance were measured.  
73

### 74 III. RESULTS

75 Figure 1(a) shows the longitudinal magnetoresistance  
76 (MR)  $\equiv (R_{xx}(B) - R_{xx}(0))/R_{xx}(0)$  of the various sam-  
77 ples considered. We find that above  $\sim 2$  T the MR in  
78 BST6 and BST7 is manifestly linear whereas the MR in  
79 BST15 and BST25 appears to be neither purely linear nor  
80 quadratic. While there is experimental evidence suggest-  
81 ing an association between linear MR and linearly disper-  
82 sive media<sup>20–22</sup>, as well as a theoretical basis for this asso-  
83 ciation<sup>23</sup>, we note that disorder can also render giant lin-  
84 ear MR<sup>24,25</sup> by admixing longitudinal and Hall voltages.  
85 In Fig. 1(b) we see that  $R_{xy}$  is linear in  $B$  and its slope  
86 changes sign from positive (BST6) to negative (BST15  
87 and BST25). This is simply a reflection of different  
88 charge carrier types of  $\text{Bi}_2\text{Te}_3$  ( $n$ -type) and  $\text{Sb}_2\text{Te}_3$  ( $p$ -  
89 type), where electrons (holes) dominate transport when  
90  $\text{Sb}_2\text{Te}_3$  is thin (thick). Intriguingly, Fig. 1(c) shows  $R_{xy}$   
91 vs  $B$  measured in two different Hall bar devices of BST7  
92 to be strongly non-linear and non-monotonic. Qualita-  
93 tively, it appears as if  $R_{xy}$  is picking up a large com-  
94 ponent of  $R_{xx}$  despite the Hall probes being aligned to  
95 each other with lithographic ( $\mu\text{m}$ -scale) precision. We

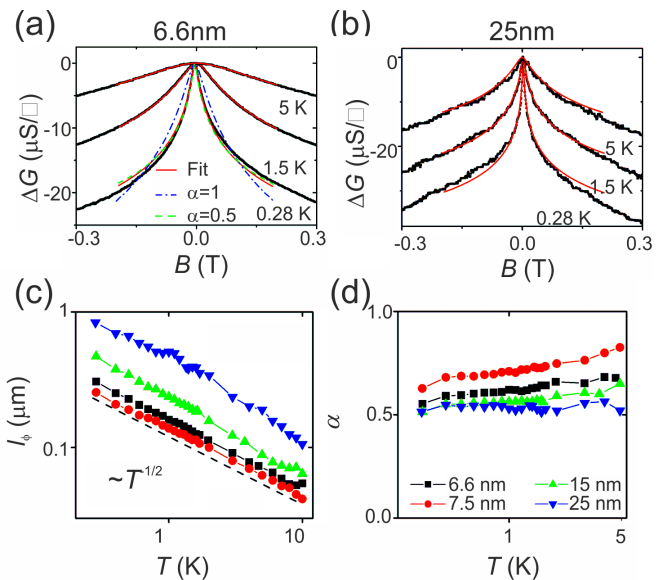


FIG. 2. (a+b) Weak antilocalization peaks for 2 different  $\text{Sb}_2\text{Te}_3$ -thicknesses and at 3 different temperatures. Fits to the measurements, based on the HLN model, are shown in straight red lines, while curves with  $\alpha$  at 0.5 (green dashed line) and 1 (blue dashed-dotted line) allow to estimate the error. (c)  $l_\phi$  as a function of  $T$  for various  $t_{\text{Sb}_2\text{Te}_3}$  in a log-log plot. All curves are proportional to  $\propto T^{-0.5}$  (dashed line) but shifted with respect to each other. (d)  $\alpha$  as a function of  $T$  for various  $t_{\text{Sb}_2\text{Te}_3}$ .

96 conjecture, therefore, that BST7 is very close to where  
97 the Hall coefficient  $R_H$  precisely changes from positive  
98 to negative. Seemingly to the contrary, ARPES mea-  
99 surements in Ref. 14 reveal that  $E_F$  intersects the Dirac  
100 point in samples with  $15 \text{ nm} < t_{\text{Sb}_2\text{Te}_3} < 25 \text{ nm}$ , in which  
101 parameter regime Fig. 1(b) indicates a net excess of  $p$ -  
102 type carriers. The investigation of this discrepancy is the  
103 major focus of this manuscript.

104 Figures 2(a+b) show the low-field MR where a pro-  
105 nounced ‘weak anti-localisation’ (WAL) cusp is visible at  
106 zero magnetic field ( $B$ ). The WAL corrections are well-  
107 described by the model of Hikami, Larkin and Nagaoka  
108 (HLN)<sup>26</sup>

$$\begin{aligned} \Delta\sigma_{xx}^{2D} &\equiv \sigma_{xx}^{2D}(B) - \sigma_{xx}^{2D}(0) \\ &= \alpha \frac{e^2}{2\pi^2\hbar} \left[ \ln \left( \frac{\hbar}{4eBl_\phi^2} \right) - \psi \left( \frac{1}{2} + \frac{\hbar}{4eBl_\phi^2} \right) \right]. \end{aligned} \quad (1)$$

109 Here  $\sigma_{xx} \equiv (L/W)R_{xx}/(R_{xx}^2 + R_{xy}^2)$  and the super-  
110 script 2D indicates that the equation is valid for a two-  
111 dimensional conducting sheet,  $\alpha$  is a parameter = 0.5 for  
112 each 2D WAL channel,  $e$  is the electronic charge,  $\hbar$  is  
113 Planck’s constant divided by  $2\pi$ ,  $l_\phi$  is the phase coher-  
114 ence length, and  $\psi$  is the digamma function.

115 Figure 2(c) shows the  $T$ -dependence of  $l_\phi$  for all sam-  
116 ples. We find that  $l_\phi \propto T^{-p/2}$ , where the exponent  $p = 1$   
117 is in line with 2D Nyquist scattering<sup>27,28</sup> due to electron-

118 electron scattering processes. The second fitting param-  
 119 eter  $\alpha$  is depicted in Fig. 2(d) and we find values consis-  
 120 tent with  $\alpha = 0.5$  (error estimates on  $\alpha$  can be found in  
 121 Fig. 2(a) and a discussion in Appendix A). This is consis-  
 122 tent with several previous reports on TI thin films<sup>9,29–31</sup>.

## 123 IV. DISCUSSION

### 124 A. 3-channel model

125 Having ascertained that the transport characteristics  
 126 of the  $\text{Bi}_2\text{Te}_3/\text{Sb}_2\text{Te}_3$  heterostructures are consistent  
 127 with conventional TI behaviour, we now proceed to un-  
 128 derstand the Hall characteristics. It is well-known that  
 129 the TIs  $\text{Bi}_2\text{Te}_3$  and  $\text{Sb}_2\text{Te}_3$  show bulk conduction in ad-  
 130 dition to the TSS. Thus, we start with a simple picture  
 131 of three independent conduction channels: bulk  $n$ - and  
 132  $p$ -type layers corresponding to the  $\text{Bi}_2\text{Te}_3$  and  $\text{Sb}_2\text{Te}_3$   
 133 layers, respectively, and a TSS on the top surface. While  
 134 in principle a TSS exists also at the interface with the  
 135 substrate, it is expected that its contribution to the con-  
 136 ductivity is largely diminished due to the strongly disor-  
 137 dered TI-substrate interface<sup>31,32</sup>. Thus as a first approx-  
 138 imation, we do not consider the bottom TSS.

139 Our starting point is the expressions for  $\sigma_{xx}$  and  $R_H$   
 140 in a multi-channel system<sup>33–35</sup>

$$\sigma_{xx} = e n_p \mu_p - e n_n \mu_n \pm e n_t \mu_t \quad (2)$$

$$R_H(t_{\text{SbTe}}) \equiv \frac{1}{e \cdot n_{\text{eff}}} = \frac{n_p \mu_p^2 - n_n \mu_n^2 \pm n_t (t_{\text{SbTe}}) \mu_t^2}{e(n_p \mu_p + n_n \mu_n + n_t (t_{\text{SbTe}}) \mu_t)} \quad (3)$$

141 Here  $n_{\text{eff}}$  is the effective carrier concentration,  $e$  is the  
 142 charge of an electron and  $-e$  is the charge of a hole, the  
 143 subscript  $n$ ,  $p$  and  $t$  signify bulk electrons, bulk holes, and  
 144 surface carriers, respectively,  $n_i$  are carrier concentra-  
 145 tions, and  $\mu_i$  represent the mobility of the charge carriers.  
 146 The  $\pm$  indicates, respectively, negative ( $t_{\text{SbTe}} < 20$  nm)  
 147 and positive charge carriers ( $t_{\text{SbTe}} > 20$  nm) in the TSS.  
 148 The following literature values for the bulk layers are as-  
 149 sumed:  $n_{\text{BiTe}} = 8 \times 10^{19} \text{ cm}^{-3}$  and  $\mu_n = 50 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$   
 150 for  $\text{Bi}_2\text{Te}_3$ <sup>7</sup> and  $n_{\text{SbTe}} = 4.5 \times 10^{19} \text{ cm}^{-3}$  and  $\mu_p =$   
 151  $300 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$  for  $\text{Sb}_2\text{Te}_3$ <sup>12,28,36</sup>. In order to compare  
 152  $n_{\text{BiTe}}$  and  $n_{\text{SbTe}}$  to the TSS carrier concentration, we con-  
 153 vert them to effective areal densities as  $n_n \equiv n_{\text{BiTe}} \cdot t_{\text{BiTe}}$   
 154 and  $n_p \equiv n_{\text{SbTe}} \cdot t_{\text{SbTe}}$ . It can be shown that  $n_t \propto E_B^2$   
 155 where  $E_B$  is the difference between  $E_F$  and Dirac point  
 156 (see Eq. B3, Appendix B) and  $E_B$ , in turn, can be re-  
 157 trieved from ARPES measurements in Ref.<sup>14</sup>.  $\mu_t$  is used  
 158 as a fitting parameter.

159 Figure 3(a) shows  $R_H$  as predicted by the model us-  
 160 ing the above parameters to be in good agreement with  
 161 the measured values. However, for the same paramet-  
 162 ers we find that  $R_{xx} \equiv (L/W)\sigma_{xx}$  is significantly under-  
 163 estimated especially for low  $t_{\text{SbTe}}$  (Fig. 3(b)). A likely

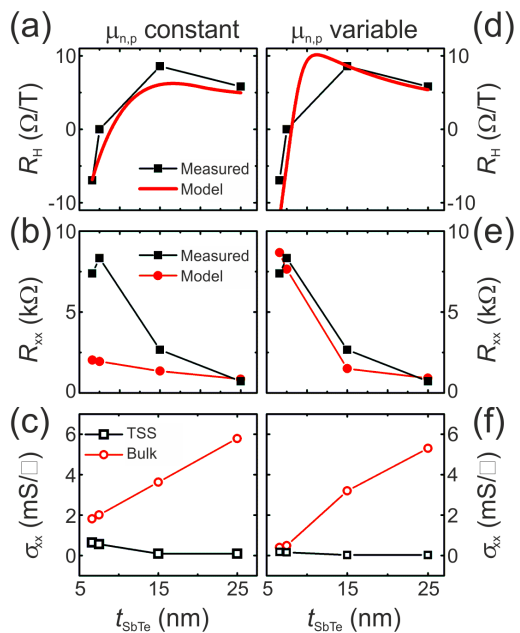


FIG. 3. (a+d) Hall slopes  $R_H$  determined from the Hall mea-  
 surements in Fig. 1(b) (black square), and fitted using Eq. 3  
 (red lines). The bulk mobilities  $\mu_{n,p}$  were kept constant in (a)  
 and reduced for low thicknesses in (d). (b+c) Comparison of  
 measured (black squares) and calculated total resistance (red  
 disks), and conductivity of the TSS (black open squares) and  
 of the bulk (red open disks), using fitting parameters from  
 (a). (e+f) Same as (b+c) but using fitting parameter from  
 (d). All variables are a function of  $t_{\text{SbTe}}$ .

164 source of this discrepancy is that the bulk  $\mu_i$  values are  
 165 not applicable for the ultra-thin films. This is especially  
 166 so considering the fact that a depletion zone will form  
 167 at the  $p$ - $n$  interface. Determining the exact profile of  
 168 the charge carrier density at the interface is beyond the  
 169 scope of this paper and instead, we demonstrate that an  
 170 *ad-hoc* thickness-dependent reduction of  $\mu_i$  of the *bulk*  
 171 layers with all other parameters unchanged, can signifi-  
 172 cantly improve the quality of the predictions. Figure 3(d)  
 173 shows the result of a fit in which  $\mu_p$  and  $\mu_n$  are reduced to  
 174 20% of their bulk value in BST6 and BST7, and to 95%  
 175 of their bulk value in BST15 and BST25. Not only do we  
 176 obtain excellent agreement with the  $R_H$  data, the model  
 177 is also able to accurately predict  $R_{xx}$  (Fig. 3(e)). The ob-  
 178 tained value of  $\mu_t = 281 \pm 17 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$  is well within  
 179 the range of previous studies in ultra-thin TIs where the  
 180 TSS dominate transport<sup>11</sup>.

181 Figure 3(f) shows the important physical insight we ar-  
 182 rive at on the basis of this simple model: the bulk contri-  
 183 bution is drastically reduced in thin films (see Fig. 3(c)),  
 184 with the TSS eventually dominating the overall conduc-  
 185 tivity  $\sigma_{\text{tot}}$  (see Fig. 3(f)).

186 To test this conclusion we measure samples with top-  
 187 gate electrodes which enable the tuning of the Fermi level  
 188  $E_F$  via a gate voltage  $V_G$ . A variation of  $E_F$  should  
 189 lead to perceptible changes of the transport properties

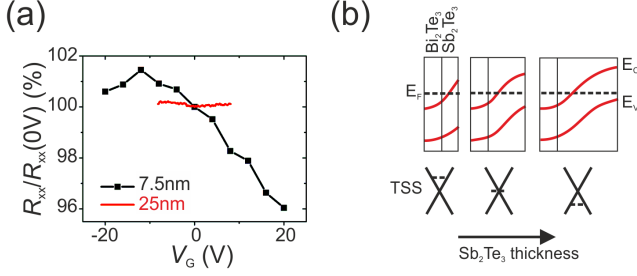


FIG. 4. (a) Gate voltage dependence of the resistivity for BST7 (black) and BST25 (red). (b) Schematic of the change of band structure as  $t_{\text{Sb}_2\text{Te}_3}$  is increased.

of the TSS (see Fig. 4(b)) while transport through the bulk should be less affected due to screening. As can be seen in Fig. 4(a) this is indeed the case, with the resistance of the thin, TSS dominated sample much more dependent on  $V_G$  than the thick, bulk dominated sample. The resistance of the thin sample is maximized when  $V_G = -12\text{ V}$ , likely corresponding to the alignment of  $E_F$  with the Dirac point. Thus, broadly speaking, despite the basic nature of the model, it captures the essential physics and provides a consistent explanation of the dependence of the longitudinal and Hall transport components. Furthermore, the results of our calculation are

$$\mathbf{j}_{c,v}^{\parallel}(z) = \frac{2e\gamma_{e,h}m_{e,h}^*\tau_{e,h}(z)}{\tau_{p(e,h)}(z)} \mathbf{v}_{c,v}^{\parallel}[u_{c,v}(z)] \left\{ \left[ \overleftrightarrow{\boldsymbol{\mu}}_{c,v}^{\parallel}(\mathbf{B}, z) \cdot \mathbf{E} \right] \right\} \cdot \mathbf{v}_{c,v}^{\parallel}[u_{c,v}(z)] \mathcal{D}_{c,v}[u_{c,v}(z)], \quad (4)$$

where  $\gamma_{e,h} = -1$  or  $+1$  for electrons and holes, respectively,  $m_{e,h}^*$  are effective masses of electrons and holes,  $\tau_{e,h}(z)$  and  $\tau_{p(e,h)}(z)$  are bulk energy- and momentum relaxation times<sup>37</sup>, the velocity  $\mathbf{v}_{c,v}^{\parallel}(\mathbf{k}) = -\gamma_{e,h} \hbar \mathbf{k}_{\parallel} / m_{e,h}^*$  (with  $\mathbf{k}$  the wavevector and  $\mathbf{k}_{\parallel}$  the in-plane wavevector),  $u_{c,v}(z) = (\hbar k_F^{e,h})^2 / 2m_{e,h}^*$  and  $k_F^{e,h}$  are Fermi energies and wave vectors in the bulk,  $\overleftrightarrow{\boldsymbol{\mu}}_{c,v}^{\parallel}$  are mobility tensors, and  $\mathcal{D}_{c,v}[u_{c,v}(z)] = (\sqrt{u_{c,v}(z)} / 4\pi^2) (2m_{e,h}^* / \hbar^2)^{3/2}$  is the electron and hole density-of-states per spin.

Similarly, one obtains the surface current per length as

$$\mathbf{j}_s^{\pm} = \mp \frac{e\tau_s \hbar k_F^s}{\tau_{sp} v_F} \mathbf{v}_s^{\pm}(u_s) \left\{ \left[ \overleftrightarrow{\boldsymbol{\mu}}_s^{\pm}(\mathbf{B}) \cdot \mathbf{E} \right] \right\} \cdot \mathbf{v}_s^{\pm}(u_s) \rho_s(u_s), \quad (5)$$

where the  $\pm$  denote when the Fermi level lies above and below the Dirac point, respectively,  $\tau_s$  and  $\tau_{sp}$  are surface energy- and momentum relaxation times,  $k_F^s = \sqrt{4\pi n_s}$  where  $n_s$  is the areal density of surface electrons,  $v_F$  is the Fermi velocity of a Dirac cone,  $\mathbf{v}_s^{\pm}(\mathbf{k}_{\parallel}) = \pm(\mathbf{k}_{\parallel} / k_{\parallel}) v_F$ ,  $u_s = \hbar v_F k_F^s$  is the Fermi energy of a Dirac cone, and  $\rho_s(u_s) = u_s / (2\pi \hbar^2 v_F^2)$  is the surface density-of-states of a

clearly consistent with the observation of ‘no’ Hall slope in BST7.

## B. Semi-classical theory

Although our simplistic model offers useful physical insights, for a more microscopic understanding it is desirable that one is not dependent on *ad-hoc* assumptions and/or a large number of experimental parameters. In the following we present a semi-classical theory for calculating magneto-conductivity tensors of surface and bulk charge carriers in a topological  $p$ - $n$  junction using zeroth and first-order Boltzmann moment equations<sup>37</sup>. Assuming the  $p$ - $n$  interface to be in the  $x$ - $y$  plane, then under a parallel external electric field  $\mathbf{E} = (E_x, E_y, 0)$  and a perpendicular magnetic field  $\mathbf{B} = (0, 0, B)$ , the total current per length in a  $p$ - $n$  junction structure is given by  $\int_{-L_A}^{L_D} dz \left[ \mathbf{j}_c^{\parallel}(z) + \mathbf{j}_v^{\parallel}(z) \right] + \mathbf{j}_s^{\pm}$ , where  $L_D$  and  $L_A$  are the thickness of the  $p$  region (donors) and  $n$  region (acceptors), respectively. Here  $\mathbf{j}_i$  indicate the current densities with  $i = c, v$  or  $s$  for conduction band, valence band and surface, respectively. The superscript  $\parallel$  is included to emphasise that the current considered is parallel to the  $p$ - $n$  interface as is experimentally the case. The bulk current densities are given by

Dirac cone.

The bulk mobility tensors  $\overleftrightarrow{\boldsymbol{\mu}}_{c,v}^{\parallel}(\mathbf{B}, z)$  are given by

$$\overleftrightarrow{\boldsymbol{\mu}}_{c,v}^{\parallel}(\mathbf{B}, z) = \frac{\mu_0(z)}{1 + \mu_0^2(z)B^2} \begin{bmatrix} 1 & \mu_0(z)B \\ -\mu_0(z)B & 1 \end{bmatrix}, \quad (6)$$

where  $\mu_0(z) = e\gamma_{e,h}\tau_{p(e,h)}(z) / m_{e,h}^*$ . A derivation of the bulk mobility tensor can be found in Appendix D. The bulk conductivity tensor is then calculated as

$$\overleftrightarrow{\boldsymbol{\sigma}}_{c,v}^{\parallel}(\mathbf{B}) = e\gamma_{e,h} \int_{-L_A}^{L_D} dz n_{e,h}(z) \left[ \frac{\tau_{e,h}(z)}{\tau_{p(e,h)}(z)} \right] \overleftrightarrow{\boldsymbol{\mu}}_{c,v}^{\parallel}(\mathbf{B}, z). \quad (7)$$

Likewise, the surface mobility tensor is

$$\overleftrightarrow{\boldsymbol{\mu}}_s^{\pm}(\mathbf{B}) = \mp \frac{\mu_1}{1 + \mu_1^2 B^2} \begin{bmatrix} 1 & \mp \mu_1 B \\ \pm \mu_1 B & 1 \end{bmatrix}, \quad (8)$$

where  $\mu_1 = 4e_0^2 \epsilon_r^2 \hbar v_F^2 / \sigma_i e^3$ ,  $\epsilon_r$  is the host dielectric constant, and  $\sigma_i$  is the surface density of impurities. This corresponds to a surface conductivity tensor given by

$$\hat{\sigma}_s^\pm(\mathbf{B}) = e\sigma_s \left( \frac{\tau_s}{\tau_{sp}} \right) \hat{\mu}_s^\pm(\mathbf{B}). \quad (9)$$

$$\begin{aligned} \hat{\sigma}_{\text{tot}}(\mathbf{B}) &= e \hat{\mu}_v^\parallel(\mathbf{B}) N_A A_h \left[ (L_A - W_p) + \int_0^{W_p} dz \exp\left(-\frac{\beta e \bar{\mu}_h N_A}{2\epsilon_0 \epsilon_r D_h} z^2\right) \right] - e \hat{\mu}_c^\parallel(\mathbf{B}) N_D A_e \\ &\times \left[ (L_D - W_n) + \int_0^{W_n} dz \exp\left(-\frac{\beta e \bar{\mu}_e N_D}{2\epsilon_0 \epsilon_r D_e} z^2\right) \right] + e \hat{\mu}_s^\pm(\mathbf{B}) \left( \frac{\alpha_0^2}{4\pi \hbar^2 v_F^2} \right) (L_A - L)^2 A_s, \end{aligned} \quad (10)$$

where  $\alpha_0$  and  $L_0$  are constants to be determined experimentally,  $N_{D,A}$  are doping concentrations,  $W_n$  and  $W_p$  are the thicknesses of the depletion zones for donors and acceptors in a  $p$ - $n$  junction,  $\bar{\mu}_{e,h}$  are  $\mu_0(z)$  evaluated at  $n_{e,h}(z) = N_{D,A}$ ,  $D_{e,h}$  are diffusion coefficients,  $\beta = 4/3$  ( $\beta = 7/3$ ) for longitudinal (Hall) conductivity. In addition, the averaged mobilities  $\hat{\mu}_{c,v}^\parallel(\mathbf{B})$  are defined by their values of  $\tau_{p(e,h)}(z)$  at  $n_{e,h}(z) = N_{D,A}$ , and three coefficients are  $A_s = \tau_s/\tau_{sp} \approx 3/4$ ,

$$\begin{aligned} A_{e,h} &= \frac{\tau_{e,h}(z)}{\tau_{p(e,h)}(z)} \Big|_{n_{e,h}(z)=N_{D,A}} \\ &= \frac{1}{6} \left( \frac{Q_c}{k_{F,e,h}^2} \right)^2 \left[ 2 \ln \left( \frac{2k_{F,e,h}^2}{Q_c} \right) - 1 \right] \\ &= \frac{Q_c^2}{6(3\pi^2 N_{D,A})^{2/3}} \left\{ 2 \ln \left[ \frac{2(3\pi^2 N_{D,A})^{1/3}}{Q_c} \right] - 1 \right\}, \end{aligned} \quad (11)$$

where  $1/Q_c$  is the Thomas-Fermi screening length. More details on the derivation of the conductivity tensors can be found in Appendix E.

From Eq. 10 one can see that there exists a critical value of  $L_A = L^*$  at which the total Hall conductivity becomes zero, which is determined from the following quadratic equation

$$\begin{aligned} &\frac{\bar{\mu}_h^2 N_A A_h}{1 + \bar{\mu}_h^2 B^2} \left\{ (L^* - W_p) + \int_0^{W_p} dz \exp\left[-\left(\frac{7e\bar{\mu}_h N_A}{6\epsilon_0 \epsilon_r D_h}\right) z^2\right] \right\} - \frac{\bar{\mu}_e^2 N_D A_e}{1 + \bar{\mu}_e^2 B^2} \left\{ (L_D - W_n) \right. \\ &\left. + \int_0^{W_n} dz \exp\left[-\left(\frac{7e\bar{\mu}_e N_D}{6\epsilon_0 \epsilon_r D_e}\right) z^2\right] \right\} \pm \frac{\mu_1^2}{1 + \mu_1^2 B^2} \left( \frac{\alpha_0^2}{4\pi \hbar^2 v_F^2} \right) (L^* - L_0)^2 A_s = 0, \end{aligned} \quad (12)$$

where the sign  $+$  ( $-$ ) corresponds to  $L_A > L_0$  ( $L_A < L_0$ ) for the contribution of the lower (upper) Dirac cone.

We note that in arriving at the above equations we have not considered scattering between the TSS and bulk layers. Including these will modify energy-relaxation times for both bulk and surface states, although no analytical expression for these can be obtained even at low  $T$ . We leave a numerical evaluation of the problem for a later manuscript. For the purposes of this manuscript, we stress that the inclusion of this coupling only serves to modify the three coefficients  $A_e$ ,  $A_h$ , and  $A_s$ , and thus the obtained result is qualitatively unchanged. Importantly, the physical content of Eq. 12 is essentially identical to that in Eq. 3, but arrived at in a more rigorous fashion. This provides a very useful microscopic ground-

ing to Eq. 3 whilst also providing additional confidence to the physical insights drawn from the simple three-channel model.

## V. CONCLUSION

In conclusion, we have reported low- $T$  magnetotransport measurements on vertical topological  $p$ - $n$  junctions and understood the data within a three-channel model for the Hall resistance. It provides useful insights into the complex interplay of the bulk and TSS in the multi-layered TI, explains the sign change of  $R_H$  with varying  $t_{SbTe}$ , and delivers values for the mobility of the TSS of  $281 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ . We then develop a Boltzmann trans-



port theory which provides a clear microscopic foundation for our model. Our work paves the way for the study of other complex TI heterostructures<sup>29,38,39</sup>, where bulk states and TSS of different carrier types coexist. In future, our method can be applied to improved topological  $p$ - $n$  junctions in which a top and bottom TSS can form novel Dirac fermion excitonic states.

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### Appendix A: Error estimates for $\alpha$

Figure 2(a) compares the results when 1)  $\alpha$  and  $l_\phi$  were both fitting variables (red line) or 2) when  $l_\phi$  alone was used as a fitting variable and  $\alpha$  was kept constant. We find that the fit for  $\alpha = 1$  (blue dashed-dotted line) is of a significantly poorer quality, indicating clearly that the data is consistent with the existence of one WAL mode. This errors become significantly larger as  $T$  is increased (here not shown) and thus one must not over interpret the apparent increase in  $\alpha$  with  $T$  in Fig. 2(d).

### Appendix B: TSS electron density

The density of states in the dirac cone<sup>33</sup> is given by

$$g(k)dk/\frac{2\pi^2}{L} = 2\pi kdk/\frac{2\pi^2}{L} = \frac{kdk}{(2\pi/L)^2} \quad (\text{B1})$$

The relation between the binding energy  $E_B$ , i.e. the difference between the Fermi energy and the Dirac point, and the Fermi wave vector  $k_F$  is

$$E_B = \beta k_F = \hbar v_F k_F \quad (\text{B2})$$

and can be retrieved from ARPES measurements in Ref. 14, carried out using samples from the same growth process and identical material parameters. For  $E_B = 215$  meV,  $k_F \approx 0.1\text{\AA}$  (see Fig. 4(h) in Ref. 14), thus  $\beta = \frac{E_B}{k_F} = 3.44 \cdot 10^{-29}$  J m. From  $\beta$ , a Fermi velocity of  $3.26 \cdot 10^5 \frac{\text{m}}{\text{s}}$  can be derived.

The electron density of the TSS is

$$n_t = k_F^2/4\pi = \frac{E_B^2}{4\pi\beta^2} \quad (\text{B3})$$

Furthermore, the relation between  $E_B$  and the  $\text{Sb}_2\text{Te}_3$ -thickness is linear ( $dE_B/dt_{\text{SbTe}} = 1.62 \cdot 10^{-12}$  J/m, see Fig. 5) and

$$n_t = \frac{(dE_B/dt_{\text{SbTe}} \cdot t_{\text{SbTe}})^2}{4\pi\beta^2} \quad (\text{B4})$$

### Appendix C: Derivation of $R_H$ and $n_{\text{eff}}$

The force acting on charges in the TSS (index t), bulk- $\text{Sb}_2\text{Te}_3$  (p) and bulk- $\text{Bi}_2\text{Te}_3$  (n) originate from an electric field  $\vec{E}$  in  $y$ -direction and a magnetic field  $\vec{B}$  in  $x$ -direction:

$$\begin{aligned} -F_{ny} &= eE_y + ev_{nx}B_z \\ -F_{ty} &= eE_y + ev_{tx}B_z \\ F_{py} &= eE_y - ev_{px}B_z \end{aligned} \quad (\text{C1})$$

Using  $v = \frac{\mu}{e}F$  with  $\mu$  the mobility, we obtain

$$\begin{aligned} \frac{v_{ny}}{\mu_n} &= E_y + \mu_n E_x B_z \\ \frac{v_{ty}}{\mu_t} &= E_y + \mu_t E_x B_z \\ \frac{v_{py}}{\mu_p} &= E_y - \mu_p E_x B_z \end{aligned} \quad (\text{C2})$$

Furthermore, no charge current is flowing in  $y$ -direction

$$\begin{aligned} J_y &= J_n + J_t + J_p \\ &= en_n v_{ny} + en_t v_{ty} + en_p v_{py} = 0 \\ \implies n_n v_{ny} &= -(n_t v_{ty} + n_p v_{py}) \end{aligned} \quad (\text{C3})$$

Inserting the velocities in the previous equation gives

$$\begin{aligned} &n_n \mu_n (E_y + \mu_n E_x B_z) \\ &= -(n_t \mu_t (E_y + \mu_t E_x B_z) + n_p \mu_p (E_y - \mu_p E_x B_z)) \\ \implies E_y (n_n \mu_n + n_t \mu_t + n_p \mu_p) \\ &= B_z E_x (-n_n \mu_n^2 - n_t \mu_t^2 + n_p \mu_p^2) \end{aligned} \quad (\text{C4})$$

The charge current in  $x$ -direction is

$$\begin{aligned} J_x &= en_n v_{nx} + en_t v_{tx} + en_p v_{px} \\ &= (n_n \mu_n + n_t \mu_t + n_p \mu_p) e E_x \end{aligned} \quad (\text{C5})$$

$E_x$  can now be replaced, resulting in

$$\begin{aligned} &e E_y (n_n \mu_n + n_t \mu_t + n_p \mu_p)^2 \\ &= B_z J_x (-n_n \mu_n^2 - n_t \mu_t^2 + n_p \mu_p^2) \\ \implies R_H &= \frac{B_z J_x}{E_y} = \frac{-n_n \mu_n^2 - n_t \mu_t^2 + n_p \mu_p^2}{e(n_n \mu_n + n_t \mu_t + n_p \mu_p)^2} \end{aligned} \quad (\text{C6})$$

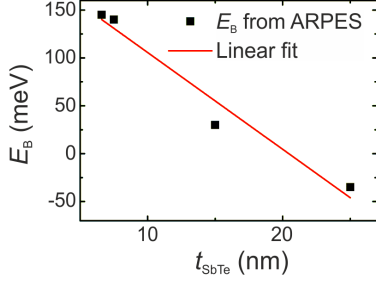


FIG. 5. Relation between  $E_B$  and  $t_{\text{SbTe}}$  (from Ref. 14)

Both  $n_p$  and  $n_t$  are depending on the thickness of the  $\text{Sb}_2\text{Te}_3$ -thickness,  $t_{\text{SbTe}}$ , with

$$n_p = n_{\text{SbTe}} \cdot t_{\text{SbTe}}$$

$$n_t(t_{\text{SbTe}}) = \frac{(dE_B/dt_{\text{SbTe}} \cdot (t_{\text{SbTe}} - t_0))^2}{4\pi\beta^2} \quad (\text{C7})$$

where  $dE_B/dt_{\text{SbTe}}$  can be gained from Fig. 5.

Thus  $R_H(t_{\text{SbTe}})$  is a function of the  $\text{Sb}_2\text{Te}_3$ -thickness of the form

$$R_H(t_{\text{SbTe}}) = \frac{-n_n(t_{\text{SbTe}})\mu_n^2 \pm n_t(t_{\text{SbTe}})\mu_t^2 + n_p\mu_p^2}{e(n_n(t_{\text{SbTe}})\mu_n + n_t(t_{\text{SbTe}})\mu_t + n_p\mu_p)^2}$$

$$= \frac{-n_{\text{SbTe}}t_{\text{SbTe}}\mu_n^2 \pm \frac{(dE_B/dt_{\text{SbTe}} \cdot (t_{\text{SbTe}} - t_0))^2}{4\pi\beta^2} \mu_t^2 + n_p\mu_p^2}{e(n_{\text{SbTe}}t_{\text{SbTe}}\mu_n + \frac{(dE_B/dt_{\text{SbTe}} \cdot (t_{\text{SbTe}} - t_0))^2}{4\pi\beta^2} \mu_t + n_p\mu_p)^2} \quad (\text{C8})$$

where the '+' sign has to be used when  $t_{\text{SbTe}} > 20$  nm and the '-' sign for  $t_{\text{SbTe}} < 20$  nm.

Because of the entity  $R_H = -1/(e \cdot n_{\text{eff}})$ , the 'effective' 2-dimensional charge density is given by

$$n_{\text{eff}} = -\frac{(n_n(t_{\text{SbTe}})\mu_n + n_t(t_{\text{SbTe}})\mu_t + n_p\mu_p)^2}{-n_n(t_{\text{SbTe}})\mu_n^2 \pm n_t(t_{\text{SbTe}})\mu_t^2 + n_p\mu_p^2} \quad (\text{C9})$$

$$\vec{\mathcal{C}} = \begin{bmatrix} 1 + q\tau_1(r_{12}B_3 - r_{13}B_2) & q\tau_1(r_{13}B_1 - r_{11}B_3) & q\tau_1(r_{11}B_2 - r_{12}B_1) \\ q\tau_2(r_{22}B_3 - r_{23}B_2) & 1 + q\tau_2(r_{23}B_1 - r_{21}B_3) & q\tau_2(r_{21}B_2 - r_{22}B_1) \\ q\tau_3(r_{32}B_3 - r_{33}B_2) & q\tau_3(r_{33}B_1 - r_{31}B_3) & 1 + q\tau_3(r_{31}B_2 - r_{32}B_1) \end{bmatrix}, \quad (\text{D4})$$

as well as the source vector  $\mathbf{s}$ , given by

$$\mathbf{s} = \begin{bmatrix} q\tau_1(r_{11}E_1 + r_{12}E_2 + r_{13}E_3) \\ q\tau_2(r_{21}E_1 + r_{22}E_2 + r_{23}E_3) \\ q\tau_3(r_{31}E_1 + r_{32}E_2 + r_{33}E_3) \end{bmatrix}, \quad (\text{D5})$$

we can reduce the linear equations to a matrix equation

$\vec{\mathcal{C}} \cdot \mathbf{v}_d = \mathbf{s}$  with a formal solution  $\mathbf{v}_d = \vec{\mathcal{C}}^{-1} \cdot \mathbf{s}$ . Explicitly, where  $\text{Det}\{\dots\}$  means taking the determinant,

## Appendix D: Bulk and surface mobility tensors

By using the force-balance equation<sup>37,40,41</sup> for bulk electrons

$$\frac{\partial \mathbf{v}_d(t|z)}{\partial t} = -\vec{\tau}_{pe}^{-1}(z) \cdot \mathbf{v}_d(t|z)$$

$$- e\vec{\mathcal{M}}_c^{-1}(z) \cdot [\mathbf{E}(t) + \mathbf{v}_d(t|z) \times \mathbf{B}(t)] = 0, \quad (\text{D1})$$

as well as the diagonal approximation for the inverse momentum-relaxation-time tensor  $\vec{\tau}_{pe}^{-1} \approx (1/\tau_j)\delta_{ij}$ , we get the following group of linear inhomogeneous equations for  $\mathbf{v}_d = \{v_1, v_2, v_3\}$

$$[1 + q\tau_1(r_{12}B_3 - r_{13}B_2)]v_1 + q\tau_1(r_{13}B_1 - r_{11}B_3)v_2 + q\tau_1(r_{11}B_2 - r_{12}B_1)v_3 = q\tau_1(r_{11}E_1 + r_{12}E_2 + r_{13}E_3),$$

$$q\tau_2(r_{22}B_3 - r_{23}B_2)v_1 + [1 + q\tau_2(r_{23}B_1 - r_{21}B_3)]v_2 + q\tau_2(r_{21}B_2 - r_{22}B_1)v_3 = q\tau_2(r_{21}E_1 + r_{22}E_2 + r_{23}E_3),$$

$$q\tau_3(r_{32}B_3 - r_{33}B_2)v_1 + q\tau_3(r_{33}B_1 - r_{31}B_3)v_2 + [1 + q\tau_3(r_{31}B_2 - r_{32}B_1)]v_3 = q\tau_3(r_{31}E_1 + r_{32}E_2 + r_{33}E_3), \quad (\text{D2})$$

where the statistically-averaged inverse effective-mass tensor for the conduction band is

$$[\vec{\mathcal{M}}_c^{-1}(z)]_{ij} \equiv \{r_{ij}\} \equiv \frac{2}{n_e(z)\mathcal{V}} \sum_{\mathbf{k}} \left[ \frac{1}{\hbar^2} \frac{\partial^2 \varepsilon_c(\mathbf{k})}{\partial k_i \partial k_j} \right] f_0[\varepsilon_c(\mathbf{k}), T; u_c(z)], \quad (\text{D3})$$

$i, j = x, y, z$ ,  $\mathbf{B} = \{B_1, B_2, B_3\}$ ,  $\mathbf{E} = \{E_1, E_2, E_3\}$ , and  $q = -e$ . By defining the coefficient matrix  $\vec{\mathcal{C}}$  for the above linear equations, i.e.,

we find the solution  $\mathbf{v}_d = \{v_1, v_2, v_3\}$  for  $j = 1, 2, 3$  as

$$v_j = \frac{\text{Det}\{\vec{\Delta}_j\}}{\text{Det}\{\vec{\mathcal{C}}\}}, \quad (\text{D6})$$

$$\begin{aligned}
\overleftrightarrow{\Delta}_1 &= \begin{bmatrix} q\tau_1(r_{11}E_1 + r_{12}E_2 + r_{13}E_3) & q\tau_1(r_{13}B_1 - r_{11}B_3) & q\tau_1(r_{11}B_2 - r_{12}B_1) \\ q\tau_2(r_{21}E_1 + r_{22}E_2 + r_{23}E_3) & 1 + q\tau_2(r_{23}B_1 - r_{21}B_3) & q\tau_2(r_{21}B_2 - r_{22}B_1) \\ q\tau_3(r_{31}E_1 + r_{32}E_2 + r_{33}E_3) & q\tau_3(r_{33}B_1 - r_{31}B_3) & 1 + q\tau_3(r_{31}B_2 - r_{32}B_1) \end{bmatrix}, \\
\overleftrightarrow{\Delta}_2 &= \begin{bmatrix} 1 + q\tau_1(r_{12}B_3 - r_{13}B_2) & q\tau_1(r_{11}E_1 + r_{12}E_2 + r_{13}E_3) & q\tau_1(r_{11}B_2 - r_{12}B_1) \\ q\tau_2(r_{22}B_3 - r_{23}B_2) & q\tau_2(r_{21}E_1 + r_{22}E_2 + r_{23}E_3) & q\tau_2(r_{21}B_2 - r_{22}B_1) \\ q\tau_3(r_{32}B_3 - r_{33}B_2) & q\tau_3(r_{31}E_1 + r_{32}E_2 + r_{33}E_3) & 1 + q\tau_3(r_{31}B_2 - r_{32}B_1) \end{bmatrix}, \\
\overleftrightarrow{\Delta}_3 &= \begin{bmatrix} 1 + q\tau_1(r_{12}B_3 - r_{13}B_2) & q\tau_1(r_{13}B_1 - r_{11}B_3) & q\tau_1(r_{11}E_1 + r_{12}E_2 + r_{13}E_3) \\ q\tau_2(r_{22}B_3 - r_{23}B_2) & 1 + q\tau_2(r_{23}B_1 - r_{21}B_3) & q\tau_2(r_{21}E_1 + r_{22}E_2 + r_{23}E_3) \\ q\tau_3(r_{32}B_3 - r_{33}B_2) & q\tau_3(r_{33}B_1 - r_{31}B_3) & q\tau_3(r_{31}E_1 + r_{32}E_2 + r_{33}E_3) \end{bmatrix}.
\end{aligned} \tag{D7}$$

373 By assuming  $r_{ij} = 0$  for  $i \neq j$ ,  $r_{jj} = 1/m_j^*$  and intro-  
374 ducing the notation  $\mu_j = q\tau_j/m_j^*$ , we find

$$\begin{aligned}
\overleftrightarrow{\mathcal{C}} &= \begin{bmatrix} 1 & -\mu_1 B_3 & \mu_1 B_2 \\ \mu_2 B_3 & 1 & -\mu_2 B_1 \\ -\mu_3 B_2 & \mu_3 B_1 & 1 \end{bmatrix}, \\
\overleftrightarrow{\Delta}_1 &= \begin{bmatrix} \mu_1 E_1 & -\mu_1 B_3 & \mu_1 B_2 \\ \mu_2 E_2 & 1 & -\mu_2 B_1 \\ \mu_3 E_3 & \mu_3 B_1 & 1 \end{bmatrix}, \\
\overleftrightarrow{\Delta}_2 &= \begin{bmatrix} 1 & \mu_1 E_1 & \mu_1 B_2 \\ \mu_2 B_3 & \mu_2 E_2 & -\mu_2 B_1 \\ -\mu_3 B_2 & \mu_3 E_3 & 1 \end{bmatrix}, \\
\overleftrightarrow{\Delta}_3 &= \begin{bmatrix} 1 & -\mu_1 B_3 & \mu_1 E_1 \\ \mu_2 B_3 & 1 & \mu_2 E_2 \\ -\mu_3 B_2 & \mu_3 B_1 & \mu_3 E_3 \end{bmatrix},
\end{aligned} \tag{D8}$$

375 and

$$\overleftrightarrow{\boldsymbol{\mu}}_c(\mathbf{B}) = -\frac{\mu_0}{1 + \mu_0^2 B^2} \begin{bmatrix} 1 + \mu_0^2 B_1^2 & -\mu_0 B_3 + \mu_0^2 B_1 B_2 & \mu_0 B_2 + \mu_0^2 B_1 B_3 \\ \mu_0 B_3 + \mu_0^2 B_2 B_1 & 1 + \mu_0^2 B_2^2 & -\mu_0 B_1 + \mu_0^2 B_2 B_3 \\ -\mu_0 B_2 + \mu_0^2 B_3 B_1 & \mu_0 B_1 + \mu_0^2 B_3 B_2 & 1 + \mu_0^2 B_3^2 \end{bmatrix}, \tag{D10}$$

384 where  $B^2 = B_1^2 + B_2^2 + B_3^2$ . By taking  $\mathbf{B} = \{0, 0, B\}$ , we  
385 find from Eq. (D10) that

$$\overleftrightarrow{\boldsymbol{\mu}}_c(\mathbf{B}) = -\frac{\mu_0}{1 + \mu_0^2 B^2} \begin{bmatrix} 1 & -\mu_0 B & 0 \\ \mu_0 B & 1 & 0 \\ 0 & 0 & 1 + \mu_0^2 B^2 \end{bmatrix}. \tag{D11}$$

386

387 For the surface case,  $E_3 = 0$ ,  $v_3 = 0$  and  $\overleftrightarrow{\mathcal{M}}_s^{-1}$ ,  $\overleftrightarrow{\boldsymbol{\tau}}_{sp}^{-1}$   
388 and  $\overleftrightarrow{\boldsymbol{\mu}}_s(\mathbf{B})$  for the  $E_s^-(\mathbf{k}_{\parallel})$  (lower-cone) state all reduce  
389 to  $2 \times 2$  tensors. This gives rise to

$$\begin{aligned}
\text{Det}\{\overleftrightarrow{\mathcal{C}}\} &= 1 + (B_1^2 \mu_2 \mu_3 + B_2^2 \mu_3 \mu_1 + B_3^2 \mu_1 \mu_2), \\
\text{Det}\{\overleftrightarrow{\Delta}_1\} &= \mu_1 E_1 + \mu_1 (B_3 E_2 \mu_2 - B_2 E_3 \mu_3) \\
&\quad + \mu_1 \mu_2 \mu_3 B_1 (\mathbf{E} \cdot \mathbf{B}), \\
\text{Det}\{\overleftrightarrow{\Delta}_2\} &= \mu_2 E_2 + \mu_2 (B_1 E_3 \mu_3 - B_3 E_1 \mu_1) \\
&\quad + \mu_1 \mu_2 \mu_3 B_2 (\mathbf{E} \cdot \mathbf{B}), \\
\text{Det}\{\overleftrightarrow{\Delta}_3\} &= \mu_3 E_3 + \mu_3 (B_2 E_1 \mu_1 - B_1 E_2 \mu_2) \\
&\quad + \mu_1 \mu_2 \mu_3 B_3 (\mathbf{E} \cdot \mathbf{B}).
\end{aligned} \tag{D9}$$

376

377 If we further assume  $m_1^* = m_2^* = m_3^* = m_e^*$  and  $\tau_1 =$   
378  $\tau_2 = \tau_3 = \tau_{pe}$ , we obtain  $\text{Det}\{\overleftrightarrow{\mathcal{C}}\} = 1 + \mu_0^2 B^2$ ,  $\text{Det}\{\overleftrightarrow{\Delta}_1\} =$   
379  $-\mu_0 E_1 + \mu_0^2 (B_3 E_2 - B_2 E_3) - \mu_0^3 B_1 (\mathbf{E} \cdot \mathbf{B})$ ,  $\text{Det}\{\overleftrightarrow{\Delta}_2\} =$   
380  $-\mu_0 E_2 + \mu_0^2 (B_1 E_3 - B_3 E_1) - \mu_0^3 B_2 (\mathbf{E} \cdot \mathbf{B})$ , and  $\text{Det}\{\overleftrightarrow{\Delta}_3\} =$   
381  $-\mu_0 E_3 + \mu_0^2 (B_2 E_1 - B_1 E_2) - \mu_0^3 B_3 (\mathbf{E} \cdot \mathbf{B})$ , where  $\mu_0 =$   
382  $e\tau_{pe}/m_e^*$ . As a result, the mobility tensor  $\overleftrightarrow{\boldsymbol{\mu}}_c(\mathbf{B})$ , which  
383 is defined through  $\mathbf{v}_d = \overleftrightarrow{\boldsymbol{\mu}}_c(\mathbf{B}) \cdot \mathbf{E}$ , can be written as

$$\overleftrightarrow{\boldsymbol{\mu}}_s(\mathbf{B}) = \frac{\mu_1}{1 + \mu_1^2 B^2} \begin{bmatrix} 1 & \mu_1 B \\ -\mu_1 B & 1 \end{bmatrix}, \tag{D12}$$

390 where  $\mu_1 = e\tau_{sp}v_F/(\hbar k_F^s)$ ,  $k_F^s = \sqrt{4\pi\sigma_s}$  and  $\sigma_s$  is the  
391 areal density of surface electrons.

### 392 Appendix E: Bulk and surface conductivity tensors

393 Under a parallel external electric field  $\mathbf{E} = (E_x, E_y, 0)$   
394 and a perpendicular magnetic field  $\mathbf{B} = (0, 0, B)$ , the to-  
395 tal parallel current per length in a  $p$ - $n$  junction structure  
396 is given by  $\int_{-L_A}^{L_D} dz [\mathbf{j}_c^{\parallel}(z) + \mathbf{j}_v^{\parallel}(z)] + \mathbf{j}_s^{\pm}$ , where  $L_D$  and  
397  $L_A$  are the distribution ranges for donors and acceptors,  
398 respectively. Here, by using the second-order Boltzmann  
399 moment equation<sup>42</sup>, the bulk current densities are found  
400 to be



$$\mathbf{j}_{c,v}^{\parallel}(z) = \frac{2e\gamma_{e,h}m_{e,h}^*\tau_{e,h}(z)}{\tau_{p(e,h)}(z)} \mathbf{v}_{c,v}^{\parallel}[u_{c,v}(z)] \left\{ \left[ \hat{\boldsymbol{\mu}}_{c,v}^{\parallel}(\mathbf{B}, z) \cdot \mathbf{E} \right] \right\} \cdot \mathbf{v}_{c,v}^{\parallel}[u_{c,v}(z)] \mathcal{D}_{c,v}[u_{c,v}(z)] , \quad (\text{E1})$$

401 where  $\mathcal{D}_{c,v}[u_{c,v}(z)] = (\sqrt{u_{c,v}(z)}/4\pi^2) (2m_{e,h}^*/\hbar^2)^{3/2}$  is  
 402 the electron and hole density-of-states per spin,  $u_{c,v}(z) =$   
 403  $(\hbar k_F^{e,h})^2/2m_{e,h}^*$  and  $k_F^{e,h}$  are Fermi energies and wave vec-  
 404 tors in a bulk,  $m_{e,h}^*$  are effective masses of electrons and  
 405 holes,  $\tau_{e,h}(z)$  and  $\tau_{p(e,h)}(z)$  are bulk energy- and momen-  
 406 tum relaxation times,<sup>37,40,41</sup>  $\mathbf{v}_{c,v}^{\parallel}(\mathbf{k}) = -\gamma_{e,h} \hbar \mathbf{k}_{\parallel}/m_{e,h}^*$ ,  
 407 and  $\gamma_{e,h} = -1$  (electrons) and  $+1$  (holes), respectively.  
 408 Similarly, the surface current per length is<sup>42</sup>

$$\mathbf{j}_s^{\pm} = \mp \frac{e\tau_s \hbar k_F^s}{\tau_{sp} v_F} \mathbf{v}_s^{\pm}(u_s) \left\{ \left[ \hat{\boldsymbol{\mu}}_s^{\pm}(\mathbf{B}) \cdot \mathbf{E} \right] \right\} \cdot \mathbf{v}_s^{\pm}(u_s) \rho_s(u_s) , \quad (\text{E2})$$

409 where  $\rho_s(u_s) = u_s/(2\pi\hbar^2 v_F^2)$  and  $u_s = \hbar v_F k_F^s$  are the  
 410 surface density-of-states and Fermi energy,  $k_F^s = \sqrt{4\pi\sigma_s}$ ,  
 411  $v_F$  is the Fermi velocity of a Dirac cone,  $\tau_s$  and  $\tau_{sp}$  are  
 412 surface energy- and momentum relaxation times,<sup>37,40,41</sup>

and  $\mathbf{v}_s^{\pm}(\mathbf{k}_{\parallel}) = \pm(\mathbf{k}_{\parallel}/k_{\parallel}) v_F$ .

413 From Eq. (E1), we find the bulk conductivity tensor as

$$\hat{\boldsymbol{\sigma}}_{c,v}^{\parallel}(\mathbf{B}) = e\gamma_{e,h} \int_{-L_A}^{L_D} dz n_{e,h}(z) \left[ \frac{\tau_{e,h}(z)}{\tau_{p(e,h)}(z)} \right] \hat{\boldsymbol{\mu}}_{c,v}^{\parallel}(\mathbf{B}, z) . \quad (\text{E3})$$

415 On the other hand, from Eq. (E2) we get the surface  
 416 conductivity tensor, given by

$$\hat{\boldsymbol{\sigma}}_s^{\pm}(\mathbf{B}) = e\sigma_s \left( \frac{\tau_s}{\tau_{sp}} \right) \hat{\boldsymbol{\mu}}_s^{\pm}(\mathbf{B}) . \quad (\text{E4})$$

417 Therefore, the total conductivity tensor  $\hat{\boldsymbol{\sigma}}_{tot}(\mathbf{B}) =$   
 418  $\hat{\boldsymbol{\sigma}}_c^{\parallel}(\mathbf{B}) + \hat{\boldsymbol{\sigma}}_v^{\parallel}(\mathbf{B}) + \hat{\boldsymbol{\sigma}}_s^{\pm}(\mathbf{B})$  can be obtained from

$$\begin{aligned} \hat{\boldsymbol{\sigma}}_{tot}(\mathbf{B}) = & e \hat{\boldsymbol{\mu}}_v^{\parallel}(\mathbf{B}) N_A A_h \left[ (L_A - W_p) + \int_0^{W_p} dz \exp\left(-\frac{\beta e \bar{\mu}_h N_A}{2\epsilon_0 \epsilon_r D_h} z^2\right) \right] \\ & - e \hat{\boldsymbol{\mu}}_c^{\parallel}(\mathbf{B}) N_D A_e \left[ (L_D - W_n) + \int_0^{W_n} dz \exp\left(-\frac{\beta e \bar{\mu}_e N_D}{2\epsilon_0 \epsilon_r D_e} z^2\right) \right] + e \hat{\boldsymbol{\mu}}_s^{\pm}(\mathbf{B}) \left( \frac{\alpha_0^2}{4\pi\hbar^2 v_F^2} \right) (L_A - L_0)^2 A_s , \quad (\text{E5}) \end{aligned}$$

419 where  $\alpha_0$  and  $L_0$  are constants to be determined exper-  
 420 imentally,  $N_{D,A}$  are doping concentrations,  $W_n$  and  $W_p$   
 421 are depletion ranges for donors and acceptors in a  $p$ - $n$   
 422 junction,  $\bar{\mu}_{e,h}$  are  $\mu_0(z)$  evaluated at  $n_{e,h}(z) = N_{D,A}$ ,  
 423  $D_{e,h}$  are diffusion coefficients, and  $\beta = 4/3$  ( $\beta = 7/3$ )  
 424 for longitudinal (Hall) conductivity. In addition, the av-  
 425 eraged mobilities  $\hat{\boldsymbol{\mu}}_{c,v}^{\parallel}(\mathbf{B})$  are defined by their values of  
 426  $\tau_{p(e,h)}(z)$  at  $n_{e,h}(z) = N_{D,A}$ , and three introduced coef-  
 427 ficients are  $A_s = \tau_s/\tau_{sp} \approx 3/4$ ,

$$\begin{aligned} A_{e,h} = & \frac{\tau_{e,h}(z)}{\tau_{p(e,h)}(z)} \Big|_{n_{e,h}(z)=N_{D,A}} \\ = & \frac{1}{6} \left( \frac{Q_c}{k_F^{e,h}} \right)^2 \left[ 2 \ln \left( \frac{2k_F^{e,h}}{Q_c} \right) - 1 \right] \\ = & \frac{Q_c^2}{6(3\pi^2 N_{D,A})^{2/3}} \left\{ 2 \ln \left[ \frac{2(3\pi^2 N_{D,A})^{1/3}}{Q_c} \right] - 1 \right\} , \quad (\text{E6}) \end{aligned}$$

where  $1/Q_c$  is the Thomas-Fermi screening length.

428 In addition, the bulk energy-relaxation times  $\tau_{e,h}(z)$   
 429 are calculated as<sup>37,40,41</sup>

$$\begin{aligned} \frac{1}{\tau_{e,h}(z)} = & \left[ \frac{2n_i}{n_{e,h}(z)\pi\hbar Q_c^2} \right] \left( \frac{e^2}{\epsilon_0 \epsilon_r} \right)^2 \times \\ & \int_0^{k_F^{e,h}(z)} dk \mathcal{D}_{c,v}(\epsilon_k^{c,v}) \left( \frac{4k^2}{4k^2 + Q_c^2} \right) \\ = & \left[ \frac{n_i m_{e,h}^*}{8n_{e,h}(z)\pi^3 \hbar^3 Q_c^2} \right] \left( \frac{e^2}{\epsilon_0 \epsilon_r} \right)^2 \times \\ & \left\{ [2k_F^{e,h}(z)]^2 - Q_c^2 \ln \left( \frac{[2k_F^{e,h}(z)]^2 + Q_c^2}{Q_c^2} \right) \right\} , \quad (\text{E7}) \end{aligned}$$

431 and the surface energy-relaxation time  $\tau_s$  is found to  
 432 be<sup>37,40,41</sup>

$$\frac{1}{\tau_s} = \frac{2\sigma_i}{\pi^2 \sigma_s \hbar^2 v_F} \left( \frac{e^2}{2\epsilon_0 \epsilon_r} \right)^2 \times \int_0^{\pi} d\phi \int_0^{k_F^s} \frac{k_{\parallel}^2 dk_{\parallel}}{(q_c + 2k_{\parallel} |\cos \phi|)^2} , \quad (\text{E8})$$

433 where  $n_i$  and  $\sigma_i$  are the impurity concentration and sur-

face density, respectively.

434  
435 Finally, the bulk chemical potentials for electrons  
436  $[u_c(z)]$  and holes  $[u_v(z)]$  are calculated as

$$[u_{c,v}(z)]^{3/2} = 3\pi^2 \left( \frac{\hbar^2}{2m_{e,h}^*} \right)^{3/2} n_{e,h}(z), \quad (\text{E9})$$

437 and the carrier density functions are

$$n_{e,h}(z) = N_{D,A} \times \exp \left\{ -\gamma_{e,h} \left( \frac{\bar{\mu}_{e,h}}{D_{e,h}} \right) \left[ \Phi(z) + \gamma_{e,h} (E_F^{e,h}/e) \right] \right\}. \quad (\text{E10})$$

438 Here, the expression for the introduced potential function

439  $\Phi(z)$  is given by

$$\Phi(z) = \begin{cases} -E_F^h/e, & z < -W_p \\ -E_F^h/e + (eN_A/2\epsilon_0\epsilon_r)(z + W_p)^2, & -W_p < z < 0 \\ E_F^e/e - (eN_D/2\epsilon_0\epsilon_r)(W_n - z)^2, & 0 < z < W_n \\ E_F^e/e, & z > W_n \end{cases}, \quad (\text{E11})$$

440 and  $E_F^e$  ( $E_F^h$ ) is the Fermi energy of electrons (holes) at  
441 zero temperature and defined far away from the depletion  
442 region.

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