This is the accepted manuscript made available via CHORUS. The article has been published as:

Disentangling surface and bulk transport in topological insulator p-n junctions
Dirk Backes, Danhong Huang, Rhodri Mansell, Martin Lanius, Jörn Kampmeier, David Ritchie, Gregor Mussler, Godfrey Gumbs, Detlev Grützmacher, and Vijay Narayan
Phys. Rev. B 96, 125125 — Published 18 September 2017
DOI: 10.1103/PhysRevB.96.125125
Disentangling surface and bulk transport in topological insulator $p$-$n$ junctions

Dirk Backes,1,* Danhong Huang,2 Rhodil Mansell,1 Martin Lanius,3 Jörn Kampmeier,3 David Ritchie,1 Gregor Mussler,3 Godfrey Gumbs,4 Detlev Grützmacher,3 and Vijay Narayan1,†

1 Cavendish Laboratory, University of Cambridge, J. J. Thomson Avenue, Cambridge CB3 0HE, United Kingdom
2 Air Force Research Laboratory, Space Vehicles Directorate, Kirtland Air Force Base, New Mexico 87117, USA
3 Peter Grünberg Institute (PGI-9), Forschungszentrum Jülich, 52425 Jülich, Germany
4 Department of Physics and Astronomy, Hunter College of the City University of New York, 695 Park Avenue, New York, New York 10065, USA

(Dated: August 21, 2017)

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 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.

PACS numbers: 73.20.-r, 73.25.+i, 73.50.-h

I. INTRODUCTION

Topological insulators (TIs) are bulk insulators with exotic ‘topological surface states’ (TSS) which are robust to backscattering from non-magnetic impurities, exhibit spin-momentum locking2 and have a Dirac-like dispersion3–5. 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$5 and $\text{Bi}_2\text{Se}_2$2,3 is that the Fermi level $E_F$ intersects the conduction/valence bands, thus giving rise to finite conductance 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 gating6–9, doping10–12, or, as recently reported, by creating $p$-$n$ junctions from two different TI films13,14.

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 problem12,15. Furthermore, and in sharp contrast to doped TIs, the intrinsic $p$ and $n$ character of the individual layers presents remarkable opportunities towards the observation of novel physics including Klein tunneling16,17, spin interference effects at the $p$-$n$ interface18, and topological exciton condensates19. 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 $(\text{Bi}_{1-x}\text{Sb}_x)_2\text{Te}_3$-$p$-$n$-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 $t_{\text{Bi}2\text{Te}3}$ = 6 nm while the top $\text{Sb}_2\text{Te}_3$ layers had thicknesses $t_{\text{Sb}2\text{Te}3}$ = 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 $W = 200$ µm and length $L = 1000$ µm using photolithography as a mask for ion milling, and Ti/Au contact pads were deposited for electrical contact.
measurements were carried out using lock-in techniques in a He-3 cryostat with a base temperature of 280 mK and a 10 T superconducting magnet. Both longitudinal ($R_{xx}$) and transverse ($R_{xy}$) components of resistance were measured.

### III. RESULTS

Figure 1(a) shows the longitudinal magnetoresistance (MR) $\equiv (R_{xx}(B) - R_{xx}(0))/R_{xx}(0)$ of the various samples considered. We find that above ~ 2 T the MR in BST6 and BST7 is manifestly linear whereas the MR in BST15 and BST25 appears to be neither purely linear nor quadratic. While there is experimental evidence suggesting an association between linear MR and linearly dispersive media,$^{20–22}$ as well as a theoretical basis for this association,$^{23}$ we note that disorder can also render giant linear MR$^{24,25}$ by admixing longitudinal and Hall voltages. In Fig. 1(b) we see that $R_{xy}$ is linear in $B$ and its slope changes sign from positive (BST6) to negative (BST15 and BST25). This is simply a reflection of different charge carrier types of Bi$_2$Te$_3$ (n-type) and Sb$_2$Te$_3$ (p-type), where electrons (holes) dominate transport when Sb$_2$Te$_3$ is thin (thick). Intriguingly, Fig. 1(c) shows $R_{xy}$ vs $B$ measured in two different Hall bar devices of BST7 to be strongly non-linear and non-monotonic. Qualitatively, it appears as if $R_{xy}$ is picking up a large component of $R_{xx}$ despite the Hall probes being aligned to each other with lithographic ($\mu$m-scale) precision. We conjecture, therefore, that BST7 is very close to where the Hall coefficient $R_H$ precisely changes from positive to negative. Seemingly to the contrary, ARPES measurements in Ref. 14 reveal that $E_F$ intersects the Dirac point in samples with 15 nm $< t_{SbTe} < 25$ nm, in which parameter regime Fig. 1(b) indicates a net excess of p-type carriers. The investigation of this discrepancy is the major focus of this manuscript.

Figures 2(a+b) show the low-field MR where a pronounced ‘weak anti-localisation’ (WAL) cusp is visible at zero magnetic field ($B$). The WAL corrections are well-described by the model of Hikami, Larkin and Nagaoka (HLN)$^{26}$

$$\Delta \sigma_{2D} \equiv \sigma_{2D}(B) - \sigma_{2D}(0)$$

$$= \alpha \frac{e^2}{2\pi^2\hbar} \ln \left( \frac{\hbar}{4eB\phi} \right) - \psi \left( \frac{1}{2} + \frac{\hbar}{4eB\phi} \right).$$

(1)

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

Figure 2(c) shows the $T$-dependence of $\phi$ for all samples. We find that $T_\phi \propto T^{-p/2}$, where the exponent $p = 1$ is in line with 2D Nyquist scattering$^{27,28}$ due to electron-
electron scattering processes. The second fitting parameter $\alpha$ is depicted in Fig. 2(d) and we find values consistent with $\alpha = 0.5$ (error estimates on $\alpha$ can be found in Fig. 2(a) and a discussion in Appendix A). This is consistent with several previous reports on TI thin films.

### IV. DISCUSSION

#### A. 3-channel model

Having ascertained that the transport characteristics of the Bi$_2$Te$_3$/Sb$_2$Te$_3$ heterostructures are consistent with conventional TI behaviour, we now proceed to understand the Hall characteristics. It is well-known that the TIs Bi$_2$Te$_3$ and Sb$_2$Te$_3$ show bulk conduction in addition to the TSS. Thus, we start with a simple picture of three independent conduction channels: bulk $n$- and $p$-type layers corresponding to the Bi$_2$Te$_3$ and Sb$_2$Te$_3$ layers, respectively, and a TSS on the top surface. While in principle a TSS exists also at the interface with the substrate, it is expected that its contribution to the conductivity is largely diminished due to the strongly disordered TI-substrate interface.

Our starting point is the expressions for $\sigma_{xx}$ and $R_H$ in a multi-channel system:

$$\sigma_{xx} = e \nu_n \mu_n - e \nu_p \mu_p \pm e \nu_t \mu_t$$

$$R_H(t_{\text{BiTe}}) \equiv \frac{1}{\nu_n \mu_n} + \frac{1}{\nu_p \mu_p} + \frac{1}{\nu_t \mu_t}$$

Here $n_{\text{eff}}$ is the effective carrier concentration, $e$ is the charge of an electron and $-e$ is the charge of a hole, the subscript $n, p, t$ signify bulk electrons, bulk holes, and surface carriers, respectively, $n_t$ are carrier concentrations, and $\mu_n, \mu_p, \mu_t$ represent the mobility of the charge carriers.

The $\pm$ indicates, respectively, negative ($t_{\text{BiTe}} < 20 \text{ nm}$) and positive charge carriers ($t_{\text{BiTe}} > 20 \text{ nm}$) in the TSS.

The following literature values for the bulk layers are assumed: $n_{\text{BiTe}} = 8 \times 10^{19} \text{ cm}^{-3}$ and $\mu_n = 50 \text{ cm}^2\text{V}^{-1}\text{s}^{-1}$ for Bi$_2$Te$_3$ and $n_{\text{SbTe}} = 4.5 \times 10^{19} \text{ cm}^{-3}$ and $\mu_p = 300 \text{ cm}^2\text{V}^{-1}\text{s}^{-1}$ for Sb$_2$Te$_3$. In order to compare $n_{\text{BiTe}}$ and $n_{\text{SbTe}}$ to the TSS carrier concentration, we convert them to effective areal densities as $n_t \equiv n_{\text{BiTe}} \cdot t_{\text{BiTe}}$ and $n_p \equiv n_{\text{SbTe}} \cdot t_{\text{SbTe}}$. It can be shown that $n_t \propto E_B^2$ where $E_B$ is the difference between $E_F$ and Dirac point (see Eq. B3, Appendix B) and $E_B$, in turn, can be retrieved from ARPES measurements in Ref. 14.

$\mu_n$ is used as a fitting parameter.

Figure 3(a) shows $R_H$ as predicted by the model using the above parameters to be in good agreement with the measured values. However, for the same parameters we find that $R_{\text{xx}} \approx (L/W)\sigma_{xx}$ is significantly underestimated especially for low $t_{\text{BiTe}}$ (Fig. 3(b)). A likely source of this discrepancy is that the bulk $\mu_i$ values are not applicable for the ultra-thin films. This is especially so considering the fact that a depletion zone will form at the $p$-$n$ interface. Determining the exact profile of the charge carrier density at the interface is beyond the scope of this paper and instead, we demonstrate that an $ad$-$hoc$ thickness-dependent reduction of $\mu_i$ of the bulk layers with all other parameters unchanged, can significantly improve the quality of the predictions. Figure 3(d) shows the result of a fit in which $\mu_p$ and $\mu_n$ are reduced to 20% of their bulk value in BST6 and BST7, and to 95% of their bulk value in BST15 and BST25. Not only do we obtain excellent agreement with the $R_H$ data, the model is also able to accurately predict $R_{\text{xx}}$ (Fig. 3(e)). The obtained value of $\mu_i = 281 \pm 17 \text{ cm}^2\text{V}^{-1}\text{s}^{-1}$ is well within the range of previous studies in ultra-thin TIs where the TSS dominate transport.

Figure 3(f) shows the important physical insight we arrive at on the basis of this simple model: the bulk contribution is drastically reduced in thin films (see Fig. 3(c)), with the TSS eventually dominating the overall conductivity $\sigma_{\text{tot}}$ (see Fig. 3(f)).

To test this conclusion we measure samples with top-gate electrodes which enable the tuning of the Fermi level $E_F$ via a gate voltage $V_G$. A variation of $E_F$ should lead to perceptible changes of the transport properties.
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. Assuming the $p$-$n$ interface to be in the $x$-$y$ plane, then under a parallel external electric field $E = (E_x, E_y, 0)$ and a perpendicular magnetic field $B = (0, 0, B)$, the total current per length in a $p$-$n$ junction structure is given by

$$j^i_{c,v}(z) = \frac{2e\gamma_{e,h}m^*_e\tau_{e,h}(z)}{\tau_{p(e,h)}(z)} v^i_{c,v}[u_{c,v}(z)] \left\{ \left[ \vec{\mu}_{c,v}^\parallel(B, z) \cdot E \right] \cdot v^i_{c,v}(u_{c,v}(z)) \right\} D_{c,v}[u_{c,v}(z)],$$

where $\gamma_{e,h} = -1$ or +1 for electrons and holes, respectively, $m^*_e$ are effective masses of electrons and holes, $\tau_{e,h}(z)$ and $\tau_{p(e,h)}(z)$ are bulk energy- and momentum relaxation times, $v^i_{c,v}(k)$ is the velocity of the $i$th kind, $k$ is the wavevector and $m^*_e$ and $m^*_h$ are Fermi energies and wave vectors in the bulk, $\mu^\parallel_{c,v}$ are mobility tensors, and $D_{c,v}(u_{c,v}(z)) = \left( \sqrt{u_{c,v}(z)/4\pi^2} \right) (2m^*_e/h^2)^{3/2} \Delta$ the electron and hole density-of-states per spin.

Similarly, one obtains the surface current per length as

$$j^\pm_u = \pm \frac{e\gamma_{e,h}k^\parallel_{e,h}}{\tau_{sp}v_F} v^\pm_u(u_s) \left\{ \left[ \vec{\mu}_{c,v}^\parallel(B) \cdot E \right] \cdot v^\pm_u(u_s) \rho_u(u_s) \right\},$$

where $\pm$ 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, $k^\parallel_{e,h} = \sqrt{4\pi m^*_e}$ is the Fermi velocity of a Dirac cone, $v^\pm_u(k) = \pm \left( k^\parallel_{e,h}/k^\parallel_{e,h} \right) v_F$, $u_s = h\nu_Fk^\parallel_{e,h}$ is the Fermi energy of a Dirac cone, and $\rho_u(u_s) = u_s/(2\pi^2v_F^2)$ is the surface density-of-states of a Dirac cone.

The bulk mobility tensors $\mu^\parallel_{c,v}(B, z)$ are given by

$$\mu^\parallel_{c,v}(B, z) = \frac{\mu_0(z)}{1 + \mu_0(z)B^2} \begin{bmatrix} 1 & \mu_0(z)B \\ -\mu_0(z)B & 1 \end{bmatrix},$$

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

$$\sigma^\parallel_{c,v}(B) = \frac{e\gamma_{e,h}}{\tau_{p(e,h)}(z)} v^i_{c,v}[u_{c,v}(z)] \left\{ \left[ \vec{\mu}_{c,v}^\parallel(B, z) \cdot E \right] \cdot v^i_{c,v}[u_{c,v}(z)] \right\} D_{c,v}[u_{c,v}(z)].$$

Likewise, the surface mobility tensor is

$$\mu^{\pm}_u(B) = \pm \frac{\mu_1}{1 + \mu_1^2B^2} \begin{bmatrix} 1 & \mp\mu_1B \\ \pm\mu_1B & 1 \end{bmatrix},$$

where $\mu_1 = 4e\epsilon_0^2\epsilon_r^2h^2/\sigma_1\epsilon^3$, $\epsilon_r$ is the host dielectric constant, and $\sigma_1$ is the surface density of impurities. This corresponds to a surface conductivity tensor given by

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{image}
\caption{(a) Gate voltage dependence of the resistivity for BST7 (black) and BST25 (red). (b) Schematic of the change of band structure as $t_{BST}$ is increased.}
\end{figure}
Therefore, the total conductivity tensor \( \vec{\sigma}_{\text{tot}}(B) = \vec{\sigma}_c(B) + \vec{\sigma}_v(B) + \vec{\sigma}_s(B) \) is obtained as

\[
\vec{\sigma}_{\text{tot}}(B) = e \vec{\mu}_e(B) N_A A_h \left[ (L_A - W_p) + \int_0^{W_p} dz \exp \left( -\frac{\beta e \mu_n N_A}{2e_0 \epsilon_r D_h} z^2 \right) \right] - e \vec{\mu}_v(B) N_D A_e \\
\times \left[ (L_D - W_n) + \int_0^{W_n} dz \exp \left( -\frac{\beta e \mu_N D}{2e_0 \epsilon_r D_c} z^2 \right) \right] + e \vec{\mu}_s(B) \left( \frac{\alpha_0^2}{4\pi \hbar^2 v_F^2} \right) (L_A - L)^2 A_s,
\]

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, \( \mu_{e,h} \) are \( \mu_0(z) \) evaluated at \( n_{e,h}(z) = N_{D,A}, D_{e,h} \) are diffusion coefficients, \( \beta = 4/3 \) for longitudinal (Hall) conductivity. In addition, the averaged mobilities \( \vec{\mu}_{e,v}(B) \) are defined by their values of \( \tau_{p(e,h)}(z) \) at \( n_{e,h}(z) = N_{D,A} \), and three coefficients are \( A_s = \tau_s/\tau_{ap} \approx 3/4, \)

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 \( A_c, A_b, \) 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-

\[ V. \text{ CONCLUSION} \]

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 multilayered TI, explains the sign change of \( R_H \) with varying \( \delta_{60Te} \) and delivers values for the mobility of the TSS of 281 cm\(^2\)V\(^{-1}\)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, 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.

ACKNOWLEDGMENTS

D.B., D.R. and V.N. acknowledge funding from the Leverhulme Trust, UK, D.B., R.M., D.R., and V.N. acknowledge funding from EPSRC (UK). DH would like to thank the support from the Air Force Office of Scientific Research (AFOSR). G.M., M.L., J.K. and D.G. acknowledge financial support from the DFG-funded priority programme SPP1666.

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 is given by

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

(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

$$E_B = \beta k_F = h\nu_F k_F$$

(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, $k_F \approx 0.1\AA$ (see Fig. 4(h) in Ref. 14), thus

$$\beta = \frac{E_B}{k_F} = 3.44 \cdot 10^{-29} \text{ J m}.$$ From $\beta$, a Fermi velocity of $3.26 \cdot 10^5 \text{ m s}^{-1}$ can be derived.

The electron density of the TSS is

$$n_t = k_F^2/4\pi = \frac{E_B}{4\pi \beta^2}$$

(B3)

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

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

(B4)

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

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

$$F_{xy} = eE_y + ev_{nx}B_z$$

$$F_{yx} = eE_y + ev_{kx}B_z$$

$$F_{py} = eE_y - ev_{px}B_z$$

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

$$\frac{v_{xy}}{\mu_n} = E_y + v_{nx}B_z$$

$$\frac{v_{yx}}{\mu_p} = E_y + v_{kx}B_z$$

$$\frac{v_{py}}{\mu_p} = E_y - v_{px}B_z$$

(C2)

Furthermore, no charge current is flowing in y-direction

$$J_y = J_n + J_k + J_p = 0$$

$$\Rightarrow n_n v_{ny} = - (n_t v_{nx} + n_p v_{py})$$

Inserting the velocities in the previous equation gives

$$n_n \mu_n (E_y + v_{nx}B_z)$$

$$= -(n_t \mu_t (E_y + v_{kx}B_z) + n_p \mu_p (E_y - v_{px}B_z))$$

$$\Rightarrow E_y (n_n \mu_n + n_t \mu_t + n_p \mu_p)$$

$$= B_z E_x (n_t \mu_t^2 + n_p \mu_p^2)$$

(C4)

The charge current in x-direction is

$$J_x = n_n v_{nx} + n_t v_{kx} + n_p v_{px}$$

$$= (n_n \mu_n + n_t \mu_t + n_p \mu_p) eE_x$$

(C5)

$E_x$ can now be replaced, resulting in

$$eE_y (n_n \mu_n + n_t \mu_t + n_p \mu_p)^2$$

$$= B_z J_x (-n_n \mu_n^2 - n_t \mu_t^2 + n_p \mu_p^2)$$

$$\Rightarrow \frac{R_H}{E_y} = \frac{B_z J_x}{e(n_n \mu_n + n_t \mu_t + n_p \mu_p)^2}$$

(C6)
Both \( n_p \) and \( n_t \) are depending on the thickness of the Sb\(_2\)Te\(_3\)-thickness, \( t_{\text{SbTe}} \), with

\[
\frac{n_p}{n_t(t_{\text{SbTe}})} = \frac{(\frac{dE_s}{dT_{\text{SbTe}}} \cdot (t_{\text{SbTe}} - t_0))^2}{4 \pi s^2}
\]

where \( dE_s/dT_{\text{SbTe}} \) can be gained from Fig. 5.

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

\[
R_H(t_{\text{SbTe}}) = \frac{-n_s(t_{\text{SbTe}})\mu_s^2 + n_e(t_{\text{SbTe}})\mu_e^2 + n_p\mu_p^2}{e(n_s(t_{\text{SbTe}})\mu_s + n_t(t_{\text{SbTe}})\mu_t + n_p\mu_p)^2}
\]

where the ‘+’ sign has to be used when \( t_{\text{SbTe}} > 20 \text{ nm} \) and the ‘-’ sign for \( t_{\text{SbTe}} < 20 \text{ nm} \).

Because of the entity \( R_H = -1/(\epsilon \cdot \text{n_eff}) \), the ‘effective’ 2-dimensional charge density is given by

\[
n_{\text{eff}} = \frac{(n_s(t_{\text{SbTe}})\mu_s + n_t(t_{\text{SbTe}})\mu_t + n_p\mu_p)^2}{-n_s(t_{\text{SbTe}})\mu_s^2 + n_t(t_{\text{SbTe}})\mu_t^2 + n_p\mu_p^2}
\]

as well as the source vector \( s \), given by

\[
s = \begin{bmatrix}
q_1(12B_3 - r_{12}B_2) \\
q_2(22B_2 - r_{22}B_1) \\
q_3(32B_3 - r_{32}B_3)
\end{bmatrix}
\]

we can reduce the linear equations to a matrix equation \( \mathbf{C} \cdot \mathbf{v}_d = s \) with a formal solution \( \mathbf{v}_d = \mathbf{C}^{-1} \cdot s \). Explicitly, setting \( \det(\mathbf{C}) \) means taking the determinant.
By assuming \( r_{ij} = 0 \) for \( i \neq j \), \( r_{jj} = 1/m_j^\ast \) and introducing the notation \( \mu_j = q_j/m_j^\ast \), we find

\[
\hat{\Delta}_1 = \begin{bmatrix}
q_1(r_{11}E_1 + r_{12}E_2 + r_{13}E_3) & q_1(r_{13}B_1 - r_{11}B_3) & q_1(r_{11}B_2 - r_{12}B_1) \\
q_2(r_{21}E_1 + r_{22}E_2 + r_{23}E_3) & q_2(r_{23}B_1 - r_{21}B_3) & q_2(r_{21}B_2 - r_{22}B_1) \\
q_3(r_{31}E_1 + r_{32}E_2 + r_{33}E_3) & q_3(r_{33}B_1 - r_{31}B_3) & q_3(r_{31}B_2 - r_{32}B_1)
\end{bmatrix},
\]

\[
\hat{\Delta}_2 = \begin{bmatrix}
1 + q_1(r_{13}B_3 - r_{12}B_2) & q_1(r_{11}E_1 + r_{12}E_2 + r_{13}E_3) & q_1(r_{12}B_1 - r_{11}B_2 + r_{13}E_3) \\
q_2(r_{23}B_3 - r_{22}B_2) & q_2(r_{21}E_1 + r_{22}E_2 + r_{23}E_3) & q_2(r_{21}B_1 - r_{22}B_2) \\
q_3(r_{33}B_3 - r_{32}B_2) & q_3(r_{31}E_1 + r_{32}E_2 + r_{33}E_3) & q_3(r_{31}B_1 - r_{32}B_2)
\end{bmatrix},
\]

\[
\hat{\Delta}_3 = \begin{bmatrix}
1 + q_1(r_{13}B_3 - r_{12}B_2) & q_1(r_{12}B_1 - r_{11}B_2 + r_{13}E_3) \\
q_2(r_{23}B_3 - r_{22}B_2) & q_2(r_{21}B_1 - r_{22}B_2) \\
q_3(r_{33}B_3 - r_{32}B_2) & q_3(r_{31}B_1 - r_{32}B_2)
\end{bmatrix}.
\]

\[
\hat{\mathbf{c}} = \begin{bmatrix}
1 & -\mu_1 B_3 & \mu_1 B_2 \\
-\mu_2 B_3 & 1 & -\mu_2 B_1 \\
-\mu_3 B_3 & -\mu_3 B_1 & 1
\end{bmatrix},
\]

\[
\hat{\mathbf{\Delta}}_1 = \begin{bmatrix}
1 & \mu_1 E_1 & \mu_1 E_2 \\
\mu_2 E_1 & 1 & -\mu_2 B_1 \\
\mu_3 E_1 & \mu_3 B_1 & 1
\end{bmatrix},
\]

\[
\hat{\mathbf{\Delta}}_2 = \begin{bmatrix}
1 & \mu_1 E_1 & \mu_1 B_2 \\
\mu_2 E_2 & 1 & -\mu_2 B_1 \\
\mu_3 E_2 & \mu_3 B_1 & 1
\end{bmatrix},
\]

\[
\hat{\mathbf{\Delta}}_3 = \begin{bmatrix}
1 & -\mu_1 B_3 & \mu_1 E_1 \\
\mu_2 B_3 & 1 & \mu_2 E_2 \\
-\mu_3 B_3 & \mu_3 B_1 & 1
\end{bmatrix},
\]

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

\[
\hat{\mathbf{\mu}}_c(\mathbf{B}) = -\frac{\mu_0}{1 + \mu_0^2 B^2} \begin{bmatrix}
1 + \mu_0^2 B_1^2 & -\mu_0 B_3 + \mu_0^2 B_1 B_2 & \mu_0 B_2 + \mu_0^2 B_1 B_3 \\
-\mu_0 B_2 + \mu_0^2 B_3 B_1 & 1 + \mu_0^2 B_2^2 & -\mu_0 B_1 + \mu_0^2 B_2 B_3 \\
-\mu_0 B_3 + \mu_0^2 B_1 B_2 & -\mu_0 B_1 + \mu_0^2 B_2 B_3 & 1 + \mu_0^2 B_3^2
\end{bmatrix},
\]

and

\[
\hat{\mathbf{\mu}}_s(\mathbf{B}) = \frac{\mu_1}{1 + \mu_1^2 B^2} \begin{bmatrix}
1 & \mu_1 B \\
-\mu_1 B & 1
\end{bmatrix},
\]

where \( \mu_1 = e\tau_{sp}v_F/(\hbar k_F^3) \), \( k_F^3 = \sqrt{4\pi\sigma_s} \) and \( \sigma_s \) is the areal density of surface electrons.

**Appendix E: Bulk and surface conductivity tensors**

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 parallel current per length in a p-n junction structure is given by

\[
\int_{L_x}^{L_D} dz \left[ j_{\parallel}^B(\mathbf{z}) + j_{\parallel}^s(\mathbf{z}) \right],
\]

where \( L_D \) and \( L_x \) are the distribution ranges for donors and acceptors, respectively. Here, by using the second-order Boltzmann moment equation \( 42 \), the bulk current densities are found to be

\[
\hat{\mathbf{\mu}}_c(\mathbf{B}) = \begin{bmatrix}
\mu_{1c} & \mu_{2c}
\end{bmatrix},
\]

\[
\hat{\mathbf{\mu}}_s(\mathbf{B}) = \begin{bmatrix}
\mu_{1s} & \mu_{2s}
\end{bmatrix},
\]

where \( \mu_{1c} = e\tau_{sp}v_F/(\hbar k_F^3) \), \( k_F^3 = \sqrt{4\pi\sigma_s} \) and \( \sigma_s \) is the areal density of surface electrons.
\[ j_{c,v}^\pm (z) = \frac{2e\gamma_{c,h} m_{e,h}^* \tau_{c,h} (z)}{\tau_{p(e,h)} (z)} \mathbf{v}_{c,v}^\pm (u_{c,v} (z)) \cdot \{ \mathbf{\hat{\mu}}_{c,v}^{\parallel} (B, z) \cdot \mathbf{E} \} \cdot \mathbf{v}_{c,v}^\parallel (u_{c,v} (z)) \mathcal{D}_{c,v} [u_{c,v} (z)] , \] (E1)

and \( \mathbf{v}_s^\pm (k_i) = \pm (k_i / k_i) v_F . \)

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

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

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

\[ \sigma_s^{\pm} (B) = e \sigma_s \left( \frac{\tau_s}{\tau_{sp}} \right) \mathbf{\hat{\mu}}_s^\pm (B) . \] (E4)

Therefore, the total conductivity tensor \( \sigma_{tot} (B) = \sigma_v^{\parallel} (B) + \sigma_s^{\pm} (B) + \sigma_v^{\parallel} (B) \) can be obtained from

\[ \sigma_{tot} (B) = e \mathbf{\bar{\mu}}_c^\parallel (N_A A_h (L_A - W_p) + \int_0^W_p dz \exp \left( - \frac{\beta e \bar{\mu}_h N_A}{2 \epsilon_0 c, D_h} z \right) \right] - e \mathbf{\bar{\mu}}_c^\parallel (N_D A_e (L_D - W_n) + \int_0^W_n dz \exp \left( - \frac{\beta e \bar{\mu}_h N_D}{2 \epsilon_0 c, D_e} z \right) \right] + e \mathbf{\bar{\mu}}_s^\pm (B) \left( \frac{\alpha_0^2}{4 \pi \hbar^2 v_F} \right) (L_A - L_0)^2 A_s , \] (E5)

where \( \sigma_0 \) and \( L_0 \) are constants to be determined experimentally, \( N_{D,A} \) are doping concentrations, \( W_n \) and \( W_p \) are depletion ranges for donors and acceptors in a p-n junction, and \( \bar{\mu}_{c,h} \) are \( \mu_0 (z) \) evaluated at \( n_{c,h} (z) = N_{D,A} \), \( D_{c,h} \) are diffusion coefficients, and \( \beta = 4 / 3 \) \( (\beta = 7 / 3) \) for longitudinal (Hall) conductivity. In addition, the averaged mobilities \( \mathbf{\bar{\mu}}_{c,v}^\parallel (B) \) are defined by their values of \( \tau_{p(e,h)} (z) \) at \( n_{c,h} (z) = N_{D,A}, \) and three introduced coefficients are \( A_s = \tau_s / \tau_{sp} \approx 3 / 4 , \)

\[ A_{c,h} = \frac{\tau_{c,h} (z)}{\tau_{p(c,h)} (z)} \biggr|_{n_{c,h} (z) = N_{D,A}} = \frac{1}{6} \left( \frac{Q_c}{Q_c^2} \right)^2 \left[ 2 \ln \left( \frac{2 k_{F,h}^c}{Q_c} \right) - 1 \right] , \] (E6)

and the surface energy-relaxation time \( \tau_s \) is found to be \( \tau_s = \frac{1}{\tau_s} = \frac{2 \sigma_i}{\pi^2 \sigma_s \hbar^2 v_F} \left( \frac{e^2}{2 \epsilon_0 c, r} \right)^2 \times \int_0^\pi d\phi \int_0^{k_{F,h}^c} \frac{k_{F}^2 dk_{||}}{(q_c + 2k_{||} | cos \phi |)^2} , \] (E8)

where \( n_i \) and \( \sigma_i \) are the impurity concentration and sur-
face density, respectively.

Finally, the bulk chemical potentials for electrons
\[ [u_e(z)] \text{ and holes } [u_v(z)] \text{ are calculated as} \]
\[ [u_e(z)]^{3/2} = 3\pi^2 \left( \frac{h^2}{2m_e} \right)^{3/2} n_e(z), \quad \text{(E9)} \]
and the carrier density functions are
\[ n_{e,h}(z) = N_{D,A} \times \exp \left\{ -\gamma_{e,h} \left( \frac{\mu_{e,h}}{D_{e,h}} \right) [\Phi(z) + \gamma_{e,h}(E_F^{e,h}/e)] \right\}. \quad \text{(E10)} \]

Here, the expression for the introduced potential function
\[ \Phi(z) \text{ is given by} \]
\[ \Phi(z) = \begin{cases} -E_F^e/e, & z < -W_p, \\ -E_F^e/e + (eN_A/2\epsilon_F) (z + W_p)^2, & -W_p < z < 0, \\ E_F^e/e - (eN_D/2\epsilon_F) (W_n - z)^2, & 0 < z < W_n, \\ E_F^e/e, & z > W_n, \end{cases} \quad \text{(E11)} \]

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

---

 face density, respectively.

Finally, the bulk chemical potentials for electrons
\[ [u_e(z)] \text{ and holes } [u_v(z)] \text{ are calculated as} \]
\[ [u_e(z)]^{3/2} = 3\pi^2 \left( \frac{h^2}{2m_e} \right)^{3/2} n_e(z), \quad \text{(E9)} \]
and the carrier density functions are
\[ n_{e,h}(z) = N_{D,A} \times \exp \left\{ -\gamma_{e,h} \left( \frac{\mu_{e,h}}{D_{e,h}} \right) [\Phi(z) + \gamma_{e,h}(E_F^{e,h}/e)] \right\}. \quad \text{(E10)} \]

Here, the expression for the introduced potential function
\[ \Phi(z) \text{ is given by} \]
\[ \Phi(z) = \begin{cases} -E_F^e/e, & z < -W_p, \\ -E_F^e/e + (eN_A/2\epsilon_F) (z + W_p)^2, & -W_p < z < 0, \\ E_F^e/e - (eN_D/2\epsilon_F) (W_n - z)^2, & 0 < z < W_n, \\ E_F^e/e, & z > W_n, \end{cases} \quad \text{(E11)} \]

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

---

 face density, respectively.

Finally, the bulk chemical potentials for electrons
\[ [u_e(z)] \text{ and holes } [u_v(z)] \text{ are calculated as} \]
\[ [u_e(z)]^{3/2} = 3\pi^2 \left( \frac{h^2}{2m_e} \right)^{3/2} n_e(z), \quad \text{(E9)} \]
and the carrier density functions are
\[ n_{e,h}(z) = N_{D,A} \times \exp \left\{ -\gamma_{e,h} \left( \frac{\mu_{e,h}}{D_{e,h}} \right) [\Phi(z) + \gamma_{e,h}(E_F^{e,h}/e)] \right\}. \quad \text{(E10)} \]

Here, the expression for the introduced potential function
\[ \Phi(z) \text{ is given by} \]
\[ \Phi(z) = \begin{cases} -E_F^e/e, & z < -W_p, \\ -E_F^e/e + (eN_A/2\epsilon_F) (z + W_p)^2, & -W_p < z < 0, \\ E_F^e/e - (eN_D/2\epsilon_F) (W_n - z)^2, & 0 < z < W_n, \\ E_F^e/e, & z > W_n, \end{cases} \quad \text{(E11)} \]

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

---

 face density, respectively.

Finally, the bulk chemical potentials for electrons
\[ [u_e(z)] \text{ and holes } [u_v(z)] \text{ are calculated as} \]
\[ [u_e(z)]^{3/2} = 3\pi^2 \left( \frac{h^2}{2m_e} \right)^{3/2} n_e(z), \quad \text{(E9)} \]
and the carrier density functions are
\[ n_{e,h}(z) = N_{D,A} \times \exp \left\{ -\gamma_{e,h} \left( \frac{\mu_{e,h}}{D_{e,h}} \right) [\Phi(z) + \gamma_{e,h}(E_F^{e,h}/e)] \right\}. \quad \text{(E10)} \]

Here, the expression for the introduced potential function
\[ \Phi(z) \text{ is given by} \]
\[ \Phi(z) = \begin{cases} -E_F^e/e, & z < -W_p, \\ -E_F^e/e + (eN_A/2\epsilon_F) (z + W_p)^2, & -W_p < z < 0, \\ E_F^e/e - (eN_D/2\epsilon_F) (W_n - z)^2, & 0 < z < W_n, \\ E_F^e/e, & z > W_n, \end{cases} \quad \text{(E11)} \]

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

---

 face density, respectively.

Finally, the bulk chemical potentials for electrons
\[ [u_e(z)] \text{ and holes } [u_v(z)] \text{ are calculated as} \]
\[ [u_e(z)]^{3/2} = 3\pi^2 \left( \frac{h^2}{2m_e} \right)^{3/2} n_e(z), \quad \text{(E9)} \]
and the carrier density functions are
\[ n_{e,h}(z) = N_{D,A} \times \exp \left\{ -\gamma_{e,h} \left( \frac{\mu_{e,h}}{D_{e,h}} \right) [\Phi(z) + \gamma_{e,h}(E_F^{e,h}/e)] \right\}. \quad \text{(E10)} \]

Here, the expression for the introduced potential function
\[ \Phi(z) \text{ is given by} \]
\[ \Phi(z) = \begin{cases} -E_F^e/e, & z < -W_p, \\ -E_F^e/e + (eN_A/2\epsilon_F) (z + W_p)^2, & -W_p < z < 0, \\ E_F^e/e - (eN_D/2\epsilon_F) (W_n - z)^2, & 0 < z < W_n, \\ E_F^e/e, & z > W_n, \end{cases} \quad \text{(E11)} \]

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