Supplementary Information for ‘Observation of a Spin-Orbit Gap in a One-Dimensional Quantum Wire’:

C. H. L. Quay\textsuperscript{1,2,3}, T. L. Hughes\textsuperscript{1,4}, J. A. Sulpizio\textsuperscript{1}, L. N. Pfeiffer\textsuperscript{2,5}, K. W. Baldwin\textsuperscript{2,5}, K. W. West\textsuperscript{2,5}, D. Goldhaber-Gordon\textsuperscript{1}, R. de Picciotto\textsuperscript{2,6}

\textsuperscript{1}Physics Department, Stanford University, Stanford, CA 94305-4060, USA
\textsuperscript{2}Bell Labs, Alcatel Lucent, Murray Hill, NJ 07974, USA
\textsuperscript{3}Present address: Laboratoire de Physique des Solides (CNRS UMR 8502), Bâtiment 510, Université Paris-Sud, 91405 Orsay, France.
\textsuperscript{4}Present address: Physics Department, University of Illinois Urbana-Champaign, Urbana, IL 61801, USA
\textsuperscript{5}Present address: Department of Electrical Engineering, Princeton University, Princeton, NJ 08544, USA
\textsuperscript{6}Present address: B-Nano Ltd., 2 Meir Weisgal Road, Rehovot 76326, Israel

A. Derivation of the Hamiltonian and Choice of Parameters

We begin with the four-band Luttinger model, which models the uppermost valence bands of GaAs [1]. This model, containing the heavy-hole (HH) and light-hole (LH) valence bands, is valid for large-gap III-V semiconductors with band edges at the $\Gamma$-point. For the bulk Hamiltonian we have

$$H = \frac{\hbar^2}{2m} \sum_k c_k^+ \begin{pmatrix} - (\gamma_1 + \gamma_2) k_{||}^2 - (\gamma_1 - 2\gamma_2) k_z^2 & 2\sqrt{3}\gamma_3 k_z \gamma_5 k_z & 2\sqrt{3}\gamma_5 k_z \\ 2\sqrt{3}\gamma_5 k_z & - (\gamma_1 - \gamma_2) k_{||}^2 - (\gamma_1 + 2\gamma_2) k_z^2 & 0 \\ \sqrt{3}(\gamma_2 \hat{K} + i2\gamma_3 k_z k_y) & 0 & \sqrt{3}(\gamma_2 \hat{K} + i2\gamma_3 k_z k_y) \end{pmatrix} c_k \tag{1}$$

$$k_{||}^2 = k_x^2 + k_y^2 \tag{2}$$
$$\hat{K} = k_x^2 - k_y^2 \tag{3}$$
$$k_z = k_z \pm ik_y \tag{4}$$
$$c_k = (c_{3/2k} \ c_{1/2k} \ c_{-1/2k} \ c_{-3/2k}) \tag{5}$$

Here $c_{\pm k}$ destroys a fermion in the $J_z = \sigma$ bulk band. As mentioned in the main article, we have found that the effects of bulk inversion asymmetry are very small and therefore inconsequential; we have therefore set the parameter $C$ in Reference [1] to zero to
simplify the representation. The quantum well growth directions are the crystal [001] and [110] directions so we will rotate our axes around the [001] direction by an angle of \(-\pi/4\). From here on the x, y directions will be aligned along the [1̅0] and [110] crystal directions respectively.

In our device, holes are confined in the y and z direction, to create a 1D wire along x. Therefore, \(k_x^2\) and \(k_z^2\) may be replaced by their expectation value in the lowest subband:

\[
\langle k_a^2 \rangle \sim (\pi / d_a^2)
\]

where \(d_a\) is the confinement width in the \(a\) direction. Ignoring structural inversion asymmetry (SIA) terms, the effective 1D Hamiltonian is:

\[
H_{1d} = \frac{\hbar^2}{2m} \sum_k c_k^+ \begin{pmatrix}
-\left(\gamma_1 + \gamma_2\right)k_x^2 & 0 & -i\sqrt{3}\gamma_2k_x^2 - \beta_y \\
0 & -\left(\gamma_1 - \gamma_2\right)k_x^2 - \Delta & 0 \\
-i\sqrt{3}\gamma_2k_x^2 - \beta_y & 0 & -\left(\gamma_1 + \gamma_2\right)k_x^2
\end{pmatrix} c_k
\]

with

\[
\Delta = 4\gamma_2\pi^2 \left(\frac{1}{d_z^2} - \frac{1}{2d_y^2}\right)
\]

(7)

\[
\beta_y = \sqrt{3}\gamma_2 \frac{\pi^2}{d_y}
\]

(8)

and the basis

\[
c_k = (c_{0+3/2k} \quad c_{0+1/2k} \quad c_{0-1/2k} \quad c_{0-3/2k})
\]

(9)

Here \(c_{0\pm 3/2k}\) destroys a fermion in the lowest confinement subband of the \(J_z = \sigma\) bulk band at momentum \(k\). We have chosen a pair of subbands arising from heavy-hole like states \(c_{0\pm 3/2k}\), and a pair of subbands arising from light-hole like states \(c_{0\pm 1/2k}\). Although it is not clear a priori which bulk bands would give rise the four lowest subbands, this choice is motivated by the fact that, given Equation (7), the spacing between the chosen subbands could be comparable to the inter-subband spacing of the heavy-hole-like series of subbands. Thus, the two reasonable options seemed to be either that the two lowest sub-bands should be heavy-hole-like or that one of them should be light-hole-like. Our choice of the latter is subsequently validated by our data (see main article). The parameter \(\beta_y\) arises from the confinement in the y direction [1].

We now return to the SIA (Rashba) terms. These may be deduced from symmetry, or more formally the method of invariants [1]. For spin-3/2 systems there are two allowed Rashba terms which are linear in momentum:

\[
H_{SIA} = \alpha_1 (\vec{k} \times \vec{E}) \cdot \vec{J} + \alpha_2 (\vec{k} \times \vec{E}) \cdot \vec{J}'
\]

(10)
with $\vec{J} = (J_x, J_y, J_z)$ the spin-3/2 matrices and $\vec{J}' = (J_x', J_y', J_z')$. Empirically $\alpha_2 \ll \alpha_1$, so we shall ignore the second term [1]. For the confinement electric fields we have $E_z \neq 0$ and $E_y \neq 0$ and thus the 1D Rashba term is

$$H_{1d}^R = \alpha_1 k_x \left( E_y J_z - E_z J_y \right)$$

$$= \begin{pmatrix} \frac{1}{2} r_y k_x & \frac{\sqrt{6}}{4} \phi_z r_z k_x & 0 & 0 \\ \frac{\sqrt{6}}{4} \phi_r r_z k_x & \frac{1}{2} r_y k_x & \frac{\sqrt{3}}{2} \phi_z r_z k_x & 0 \\ 0 & \frac{\sqrt{3}}{2} \phi_r r_z k_x & -\frac{1}{2} r_y k_x & \frac{\sqrt{6}}{4} \phi_z r_z k_x \\ 0 & 0 & \frac{\sqrt{6}}{4} \phi_r r_z k_x & -\frac{3}{2} r_y k_x \end{pmatrix}$$

(11)

where $r_y = \alpha_1 E_y$, $r_z = \alpha_1 E_z$ and $\phi_\pm = 1 \pm i$.

Finally, we consider terms added to the Hamiltonian to describe the effects of an applied external magnetic field. We shall ignore here orbital magnetic field effects because our magneto-conductance data does not reveal substantial shifts of the band edges with field, which are to be expected had orbital effects been important. As for the Zeeman terms, two are expected for the spin-3/2 systems:

$$H^Z = g_1 \mu_B \vec{B} \cdot \vec{J} + g_2 \mu_B \vec{B} \cdot \vec{J}'$$

Here again $g_2 \ll g_1$, and therefore the second term can be ignored [1]. In matrix form, the remaining (first) term is:

$$H^Z = g \mu_B \begin{pmatrix} \frac{1}{2} B_z & \frac{\sqrt{6}}{4} \phi_z B_\pm & 0 & 0 \\ \frac{\sqrt{6}}{4} \phi_r B_\pm & \frac{1}{2} B_z & \frac{\sqrt{3}}{2} \phi_z B_\pm & 0 \\ 0 & \frac{\sqrt{3}}{2} \phi_r B_\pm & -\frac{1}{2} B_z & \frac{\sqrt{6}}{4} \phi_z B_\pm \\ 0 & 0 & \frac{\sqrt{6}}{4} \phi_r B_\pm & -\frac{3}{2} B_z \end{pmatrix}$$

(13)

with $g$ the Landé g-factor, $\mu_B$ the Bohr magneton, $B_\pm = B_x \pm i B_y$ and $\phi_\pm = 1 \pm i$.

Our full model Hamiltonian is:

$$H = H_{1d} + H_{1d}^R + H^Z$$

(14)

We have calculated the resultant dispersion relations for these four low-lying bands using a sensible set of parameters listed below and deduced the magneto-conductance traces expected from this model. Despite the various assumptions and approximations made, this model captures faithfully most of the features in our data semi-quantitatively (see main article). One feature in our data is not captured by this model (the occurrence of a double step in addition to a dip when the magnetic field is applied in the $x$ direction, see Figures 4b and 5e); however, pointing to a particular assumption or approximation made here as the primary cause of this shortcoming is beyond the scope of this manuscript.

We now turn to the values used for the various model parameters. We have used known values where possible and the reasoning for the choices made for the remaining parameters is detailed below. The values used are:
Table 1 Parameter values used in the model.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value used in model</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\gamma_1$</td>
<td>6.85 (5.68)</td>
</tr>
<tr>
<td>$\gamma_2$</td>
<td>2.1 (1.63)</td>
</tr>
<tr>
<td>$\gamma_3$</td>
<td>2.9 (2.35)</td>
</tr>
<tr>
<td>$\chi$</td>
<td>0.05</td>
</tr>
<tr>
<td>$d_y$</td>
<td>60nm</td>
</tr>
<tr>
<td>$d_z$</td>
<td>25nm</td>
</tr>
<tr>
<td>$r_y$</td>
<td>0</td>
</tr>
<tr>
<td>$r_z$</td>
<td>23±2meV·nm</td>
</tr>
</tbody>
</table>

The $\gamma$s are crystal parameters and are well-established in the literature [1]. The numbers in brackets are for Al$_{0.324}$Ga$_{0.676}$As calculated using a linear interpolation in the virtual crystal approximation, while those not in brackets are for GaAs. The actual numbers used in the model are $\gamma_n = \chi \gamma_{n,AlGaAs} + (1 - \chi)\gamma_{n,GaAs}$ where $\chi$ represents the leakage of the confined subband wavefunction into the AlGaAs (effectively modelling deviation from an infinite potential well). We estimated $\chi$ from simulations of the wavefunction of the lowest bound state in the potential wells in both confinement directions using the program developed by Gregory Snider for this purpose [2], exploring a rather large range of possible effective masses (0.2-0.65$m_0$, where $m_0$ is the bare electron mass), guided by theoretical values given in Reference [1] and the little that is experimentally known about the effective masses in these systems [3, 4, 5]. We obtained $0 < \chi < 0.09$ and chose a value in the middle for the model. We note that $\chi$ is in any case a parameter to which our results are rather insensitive.

As noted above, $C$ in Reference [1], which has a value of 0.009271, has been set to zero as it is in any case too small to perceptibly affect the results of the model.

The remaining four parameters $d_y$, $d_z$, $r_y$, $r_z$, are used as fitting parameters. They are grouped into two two-parameter sets which are treated differently; $d_y$ and $d_z$, the confinement related parameters are constrained to reasonable values – not too different from an estimated extent of the wave function along these two directions, as explained below. We are uncertain about the values of $d_y$ and $d_z$ because while the thicknesses of the layers giving rise to the confinement are known to great accuracy, the actual extent of the wavefunctions and the precise relation of those to $d_y$ and $d_z$ are difficult to calculate. The other two parameters, $r_y$ and $r_z$, the Rashba coefficients are simply tuned to match the
model calculations to the data. The values found are in fact the first available estimates of these parameters. This is because most work on SO in the valence band of GaAs has focused on heavy holes, whereas these are the parameters relevant for the light-hole-like subbands. As noted in the main article, we find the Rashba field to be much stronger in the \( z \) direction than in the \( y \).

We have estimated the extent of the wavefunction in each direction rather crudely – by modelling two fictitious two dimensional hole gases separately, neglecting the joint effect of both confinements in the real device. The two 2DHGs were simulated using nominal growth parameters in each direction separately [3]. We found the extent of the wavefunction in \( z \) to be about 15nm, while in \( y \), we obtain about 30-35nm. The values for \( d_z \) and \( d_y \) used in the model are within a factor of two of these figures.

Finally, we note that our nonlinear transport measurements in the same device (to be published elsewhere) point to a subband spacing of about 3meV [6], which is slightly smaller than what the model predicts with the chosen parameters (~4meV, Figure 4a of the main article); we suspect that this mismatch is due to the mixing with nearby subbands (next few conductance steps), which are not considered in this model.

**B. Conductance Calculations**

The conductance traces shown in Figures 4d and e were numerically evaluated in the following manner from the dispersion relations. First, the conductance as a function of the chemical potential was obtained within a non-interacting electron model using the Landauer-Buttiker formalism. Next, the dependence of the hole density on the chemical potential was calculated, then translated into the gate voltage as a function of the chemical potential through a capacitive factor. (Here we accounted for the correction to the geometrical capacitance due to the density of states. See for example Ref. [7]. This correction was found to be small, as expected for our device geometry.) Finally, the gate voltage is related directly to the conductance.

Two additional parameters are used in this calculation: the gate voltage at pinch-off, where the wire is empty, and the geometrical capacitance, 4.25V and 20pF/m, respectively. These values were determined by matching the gate voltages both at pinch-off and at the onset of the second conductance step seen in the data. We note that the capacitance value is in good agreement with previous work on electron wires of very similar geometry [8].
C. Data at Intermediate Fields

Figures a and b show data from Figure 3 in the main text, with additional traces taken at intermediate fields (every 0.2T) showing that the features discussed in the text (arrows) develop gradually with field and are not spurious effects. Figure c shows the data in Figure b around the spin-orbit gap.