Supplementary information for: Scattering in InAs/GaSb Coupled Quantum Wells as a Probe of Higher Order Subband Hybridisation

C. S. Knox [1;2], L.H. Li [1], M.C. Rosamond[1], E.H. Linfield[1], and C.H. Marrows[2]

1 School of Electronic and Electrical Engineering, University of Leeds, Leeds LS2 9JT, United Kingdom

2 School of Physics and Astronomy, University of Leeds, Leeds LS2 9JT, United Kingdom

Behaviour of the coupled quantum well at extreme top gate biases

In the text, it was mentioned that when a top gate bias higher than +2.5 V is applied, the carrier density experiences hysteresis with the applied top gate voltage. This hysteresis is shown in Fig. S1, where an extreme, negative top gate voltage was also applied to pinch-off the InAs well.

As the top gate bias is increased from V_{Tg} = 0 V to 5 V (step 1 in Fig. S1) the carrier density increases with applied gate bias, as expected. However, as the bias is made more negative (step 2 in Fig. S1), we notice that the Hall carrier density seems to saturate once it reaches a value of V_{Tg} = -2.75 V (at a carrier density of approximately 5.0 ×10^{11} cm^{-2}). As the top gate bias is then made more negative, there is very little modulation of the electron-like carrier density, possibly due to Fermi-level pinning within the structure. When, however, a bias of V_{Tg}=-12 V is reached, the Hall resistance becomes non-linear with increasing magnetic field, indicative of two carrier transport. Within this regime, the sheet resistance reaches 110,000 Ω/sq. However, the minimum mid-gap conductivity expected for a hybridised InAs/GaSb well is e^2/h [1,2]. Therefore, we interpret this regime as a trivial band gap, formed by pinching off the InAs well.

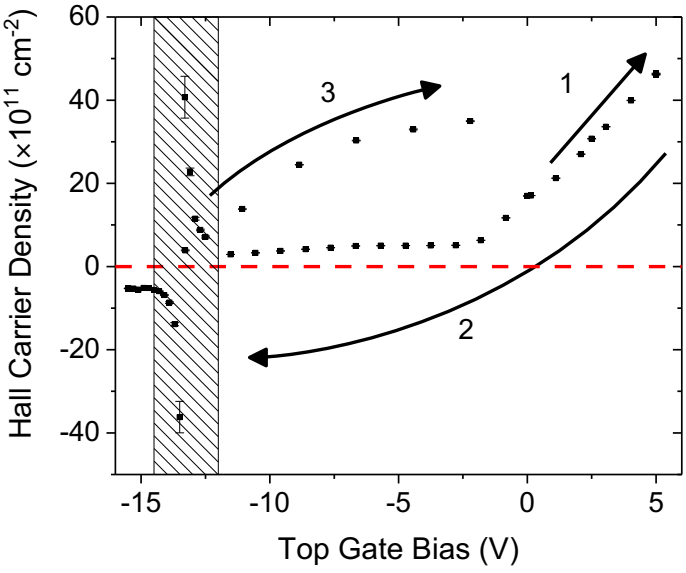

Figure S1: Low field (B <0.2 T) Hall carrier density as a function of top gate bias at very large biases, with the back gate earthed. The arrows indicate the direction and order of the gate sweeps. Zero carrier density is indicated by the dashed, red line. The shaded region indicates where the low field Hall resistance is non-linear in magnetic field, indicative of two-carrier transport.

As the bias is made yet more negative, the sign of the Hall coefficient changes, indicating that the dominant carriers within this regime are holes, rather than electrons. At the most negative biases (V_{Tg} < -14 V), the hole dominated Hall carrier density saturates at (5.21 ± 0.05) ×10^{11} cm^{-2} which we have used as an estimate for the carrier density within the GaSb well at zero bias. Finally, as the top gate bias is returned to V_{Tg} = 0 V (step 3 in Fig. S1), the carrier density returns to a much higher value than previously measured (at V_{Tg} = -6.6 V the carrier density measured in step 2 was (4.94±0.05) ×10^{11} cm^{-2}, whereas in step 3 it is found to be (30.3 ± 0.3) ×10^{11} cm^{-2}). Warming the device up to room temperature and re-cooling the sample returns the carrier density to its as-cooled state, even after these extreme biases.

Effective capacitance model

As noted in the text, the screening provided by a 2D carrier gas is never total, but can instead be modelled as a 'quantum capacitance', representing the energy cost to excite an additional carrier in a conduction channel with a given density of states. Due to this partial screening in our devices, an applied top gate bias will not only affect the InAs quantum well, but also the GaSb quantum well (and similarly the bottom gate will not only affect the GaSb channel, but also the InAs channel).

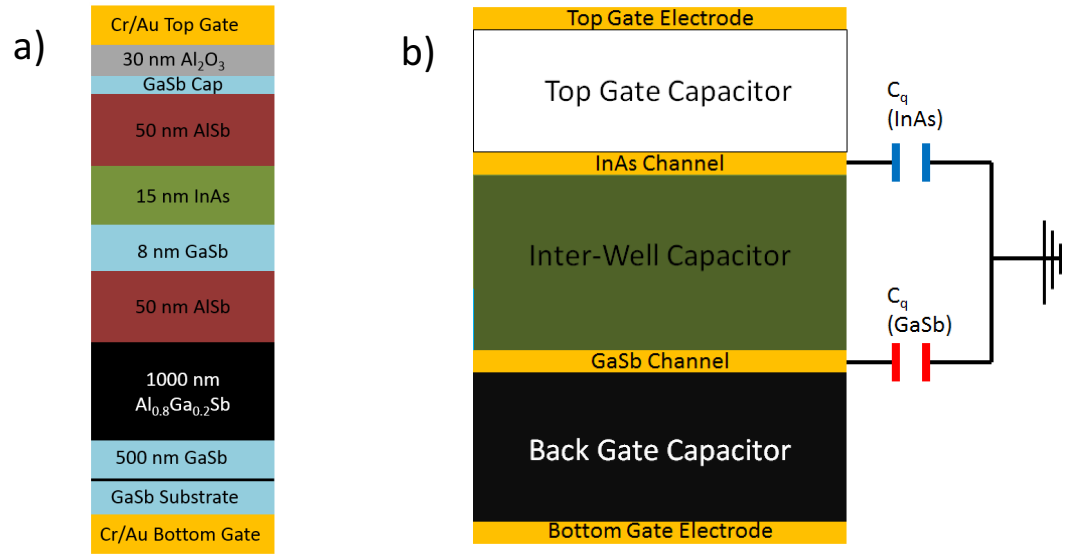

Figure S2: Schematic representations of the coupled quantum well heterostructure. a) the full stack structure, along with the related material thicknesses (as presented in Fig 1a). b) a simplified version of the stack structure used in the effective capacitance model.

These effects have been qualitatively modelled by an effective capacitance model[3]. Within this model, the conduction channels through the InAs and GaSb quantum wells are modelled as 2D sheets at the centre of their respective quantum wells. Therefore, in our stack there is an 11.5 nm gap between the two conduction channels. Given that the dielectric constants of InAs and GaSb at room temperature are 14.6 and 15.7, respectively, the capacitance per unit area of this inter-well capacitor can be estimated as 0.012 F/m^2. Additionally, if we assume that the dispersions of the InAs and GaSb wells are parabolic with respect to *k*, the quantum capacitance per unit area can be given by [4]:

$$C_q = \frac{g\, m^* e^2}{\pi \hbar},$$

where g is the number of occupied subbands and m^* is the effective mass (assumed to be $0.032m_0$ for the InAs channel and $0.4m_0$ for the GaSb channel). This results in the entire gate stack being modelled as three classical capacitors (the top gate capacitor between the top gate and the InAs channel, the inter-well capacitor formed between the two conduction channels, and the bottom gate capacitor formed between the GaSb channel and the bottom gate electrode) and two quantum capacitors, one for each conduction channel. This model is shown schematically in Fig S2. The top gate capacitor has a capacitance per unit area of 0.00111 F/m^2, and the back gate capacitor has a capacitance per unit area of 0.000102 F/m^2.

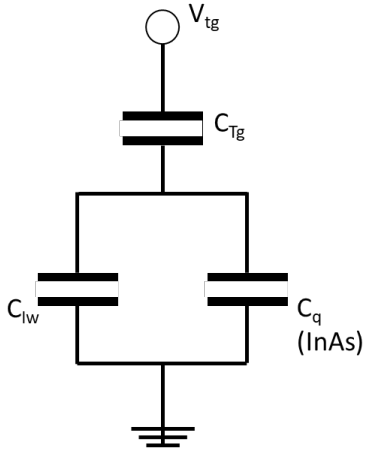

Figure S3: Effective circuit for a coupled quantum well device under a top gate bias.

To illustrate this, the equivalent circuit for a coupled quantum well device with only a top gate bias is given in Fig. S3, where C_{Tg} and C_{Iw} are the top gate and inter-well capacitors, respectively, and C_{q} (InAs) is the quantum capacitor associated with the InAs conduction channel [4]. Under an applied top gate bias, the carrier density induced in the InAs well would be:

$$n_{\mathrm{Tg}} = \frac{V_{\mathrm{Tg}}\, C_{\mathrm{Tg}}}{e},$$

(where V_{Tg} is the applied bias), ie the charge density induced across the top gate capacitor divided by the elementary charge. The carrier density of holes induced by the top gate in the GaSb well will then be proportional to the charge density induced across the inter-well capacitor

$$p_{\mathrm{Tg}=} - n_{\mathrm{Tg}} \frac{C_{\mathrm{Iw}}}{(C_{\mathrm{Iw}} + C_{\mathrm{q}}(\mathrm{InAs}))},$$

so long as the InAs well is populated. In the case where there are no electrons within the InAs channel, $C_{\mathrm{q}}(\mathrm{InAs}) = 0$, and so a top gate bias will directly modulate the hole gas within the GaSb layer.

Simplified 3×3 model of hybridised subbands

The hybridisation gap between the first electron-like subband in InAs (E1) and the highest energy heavy hole subband (H1) in GaSb has previously been modelled in detail[5], using a 4×4 matrix (equation 3.3 in supplementary Ref [5]), with the uncoupled InAs and GaSb dispersions as the diagonal elements, and complex, off-diagonal, coupling terms.

In our model we have considered the complex Hamiltonian as a block 2×2 matrix and extended it to include the second electron-like subband (E2), resulting in a Hamiltonian that can be written as

$$\begin{bmatrix} H_{E2} & 0 & \Delta \\ 0 & H_{E1} & \Delta \\ \Delta & \Delta & H_{H1} \end{bmatrix},$$

where H denotes the dispersion of the uncoupled bands, the subscripts E1, E2 and H1 refer to the relevant subbands, and Δ is the coupling term. We then simplify this model by taking Δ = 5 meV (the magnitude of the E1-H1 hybridisation gap [1]), and treating is as a constant with respect to k.

We then further simplify this model by considering the Hamiltonians of the uncoupled subbands as spin degenerate dispersions that are parabolic in k, with a fixed offset from the bottom of the uncoupled E1 subband:

$$H_x = \frac{\hbar^2 k^2}{2m_x^*} + E_{0x} + E_{\text{gate}},$$

where m^* is the effective mass of the subband (m^*=0.032 m_0 for E1 and E2 and m^*=-0.4m_0 for H1 [6]), E_0 is the energy offset from the uncoupled E1 at k=0 (E_0= 0 for E1 by definition, E_0= 0.12 eV for E2 and E_0= 0.07 eV for H1[7]) and E_{gate} is the change in energy of the subbands induced by an applied gate voltage. Numerically diagonalising this matrix at a given gate bias leads to three solutions, which we then attribute to the dispersions of the hybridised E1, E2 and H1 subbands.

A full calculation of the hybridised dispersion of the system under an applied gate bias would not only include spin-splitting effects and band non-parabolicities, but would also include the effects of the light-hole dispersion, as the inter-well coupling uses light-holes as an intermediary, which causes Δ to acquire a non-trivial k dependence [5]. Additionally, a full calculation would shed light on how Δ changes as higher order subbands (e.g. E2) couple with H1.

Supplementary References

1 I. Knez, R. R. Du, and G. Sullivan, Finite conductivity in mesoscopic Hall bars of inverted InAs/GaSb quantum wells, Phys Rev B **81**, 201301 (2010).

2 Y. Naveh and B. Laikhtman, Magnetotransport of coupled electron-holes, Europhys Lett **55**, 545 (2001).

3 F. M. Qu, et al., Electric and Magnetic Tuning Between the Trivial and Topological Phases in InAs/GaSb Double Quantum Wells, Phys Rev Lett **115**, 036803 (2015).

4 S. Luryi, Quantum Capacitance Devices, Appl Phys Lett **52**, 501 (1988).

5 S. de-Leon, L. D. Shvartsman, and B. Laikhtman, Band structure of coupled InAs/GaSb quantum wells, Phys Rev B **60**, 1861 (1999).

6 I. Vurgaftman, J. R. Meyer, and L. R. Ram-Mohan, Band parameters for III-V compound semiconductors and their alloys, J Appl Phys **89**, 5815 (2001).

7 A. Zakharova, S. T. Yen, and K. A. Chao, Strain-induced semimetal-semiconductor transition in {InAs/GaSb} broken-gap quantum wells, Phys Rev B **66**, 085312 (2002).