Low-dimensional electron transport and surface acoustic waves in GaAs and ZnO heterostructures

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This dissertation is submitted for the degree of
Doctor of Philosophy
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The work is dedicate to
my dear grandma
WANG GUANGHUI
1929–2015
Declaration

The work presented in this thesis was carried out at the Semiconductor Physics group in the Cavendish Laboratory, University of Cambridge between October 2014 and August 2018. This dissertation is the result of my own work and includes nothing which is the outcome of work done in collaboration except where specifically indicated in the text. It has not been submitted in whole or in part for any degree at this of any other university, and is less than sixty thousand words long.

Hangtian Hou
August 2018
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Abstract

A surface acoustic wave (SAW) is a combination of a mechanical wave and a potential wave propagating on the surface of a piezoelectric substrate at the speed of sound. Such waves are widely applied in not only the communication industry, but also in quantum physics research, such as nanoelectronics, spintronics, quantum optics, and even quantum information processing. Here, I focus on low-dimensional electron transport and SAWs in GaAs and ZnO semiconductor heterostructures.

The ability to pattern quantum nanostructures using gates has stimulated intense interest in research into mesoscopic physics. We have performed a series of simulations of gate structures, and having with the optimised boundary conditions and we find them to match experimental results, such as the pinch-off voltage of one-dimensional channels and SAW charge transport in induced \( n-i-n \) and \( n-i-p \) junctions. Using the improved boundary conditions, it is straightforward to model quantum devices quite accurately using standard software.

With the calculated potential, we have modelled the process how a dynamic quantum dot is driven by a SAW and have analysed error mechanisms in SAW-driven quantisation (\( I = Ne f \), where \( N \) is the number of electrons in each SAW minimum, and \( f \) is the SAW resonant frequency). From energy spectroscopy measurements, we probe the electron energy inside a SAW-driven dynamic quantum dot and find that the small addition energy, which is around 3 meV, is the main limitation for the SAW quantisation. To increase the confinement of SAW-driven quantum dots, we deposit a thin ZnO film, with a better piezoelectric coupling than GaAs, on a GaAs/AlGaAs heterostructure using high-target-utilisation sputtering (an Al\(_2\)O\(_3\) buffer layer is deposited to protect the 2DEG during sputtering). With the ZnO, the SAW amplitude is greatly improved to 100 meV and the RF power required for pumping electrons using a SAW is greatly reduced.

Finally, we have studied low-dimensional electron transport in a MgZnO/ZnO heterostructure. We have developed a technique for patterning gates using a parylene insulator, and used these to create one-dimensional quantum wires and observe electron ballistic transport with conductance quantised in units of \( 2e^2/h \). The increasing electron effective mass as the 1D electron density decreases indicates that the electron-electron interaction in this MgZnO/ZnO heterostructure is strong. Because of these strong interactions, the 0.7 anomaly is observed just below each quantised plateau, and are much stronger than in GaAs quantum wires. Furthermore, we have also calculated the SAW-modulated spontaneous and piezoelectric polarisation in the ZnO heterostructure, and have observed a sign of this SAW-modulation in 2DEG density, which is different from the classical SAW-pumping mechanism. Our results show that a ZnO heterostructure should provide a good alternative to conventional III-V semiconductors for spintronics and quantum computing as they have less nuclear spins. This paves the way for the development of qubits benefiting from the low scattering of an undoped heterostructure together with potentially long spin lifetimes.
List of publications


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Introduction and background

Since the 1980s, low-dimensional physics has stimulated great interest in research, especially in solid-state physics and nanoelectronics. With a long-term trend in the miniaturization of field-effect transistors (FET), low-dimensional electron transport has become more and more important. Here we will simply introduce low-dimensional systems and then discuss surface acoustic waves (SAWs) and their implementation in nanoelectronics, quantum optics, spintronics, and magnetoacoustics, as well as quantum information processing.

1.1 Low-dimensional systems

In a bulk metal or semiconductor, the path of electrons is easily deflected or scattered by various centres, such as defects, stable ions, and other electrons. This electron scattering makes the investigation of electron quantum transport much more difficult. Scientists have put many efforts into reducing dimensionality to investigate low-dimensional electron transport, from the two-dimensional electron gas (2DEG) to quantum dots, and experimentally observed many quantum phenomena.\(^1\text{--}^3\) Moreover, new materials have been developed, such as graphene and topological insulators (TIs). Graphene consists of a single layer of carbon atoms arranged in a hexagonal lattice, with electrons only able to move along the two-dimensional sheet.\(^3\) In three-dimensional TI material, electrons can only travel on the surface of a three-dimensional material, with very few in the bulk.\(^4\) In quantum mechanics, the density of states describes the number of available states per unit volume and energy. From three-dimensional (3D) to...
zero-dimensional (0D), the densities of states (DOS) are given by

\[ g_{3D}(E) = \frac{dn_{3D}}{dE} = \frac{8\pi \sqrt{2}}{h^3} (m^*^{3/2}) \sqrt{E - E_{\text{min}}} \]

\[ g_{2D}(E) = \frac{dn_{2D}}{dE} = \frac{4\pi m^*}{h^2} \]

\[ g_{1D}(E) = \frac{dn_{1D}}{dE} = \sqrt{\frac{2\pi m^*}{h^2}} \frac{1}{\sqrt{E - E_{\text{min}}}} \]

\[ g_{0D}(E) = \frac{dn_{0D}}{dE} = 2\delta(E - E_{\text{min}}), \]

where \( h \) is the Planck’s constant, \( m^* \) is the carrier effective mass, and \( E_{\text{min}} \) is the band minimum energy. Figure 1.1 shows the density of states in different dimensions. As the dimensionality decreases, the density of states becomes discrete, which is also one of the most important reasons why quantum phenomena can be more easily observed in low-dimensional systems.

1.1.1 Two-dimensional free electron gas

In semiconductors, a two-dimensional electron gas (2DEG) has become the most popular system for investigating low-dimensional physics. There are several methods for implementing a 2DEG in a semiconductor system. Based on modulation doping, a GaAs-based high-electron-mobility-transistor (HEMT) system has been widely used both in physics experiments and electronics industry. Moreover, field-effect induction and polarisation induction have also allowed the implementation of 2DEGs in a semiconductor heterostructure. In our work, we investigate the 2DEG in three different semiconductor heterostructures: intentionally-doped AlGaAs/GaAs heterostructures, undoped AlGaAs/GaAs heterostructures, and undoped MgZnO/ZnO heterostructures.

For example in a HEMT wafer, part of the AlGaAs layer is doped with Si atoms, which creates strong electric fields in the AlGaAs layer. By controlling the Al content in the AlGaAs layer, we can engineer the band gap. \( \text{Al}_{0.33}\text{Ga}_{0.67}\text{As} \) has an energy gap of about 1.88 eV, which is around 0.3 eV higher than that of GaAs.\(^5\) Because of the band-gap discontinuity, a potential barrier traps free electrons at the interface. In the solution to Schrödinger’s equation of an electron in a potential box:

\[ E(n, k) = \frac{\hbar^2 (k_x^2 + k_y^2 + k_z^2)}{2m^*}, \]

where \( k_z = (\pi n)/L \) and \( L \) is the confinement length in the z-direction and \( n = 1, 2, 3 \cdots \). A small \( L \) confines electrons in the ground state in z-direction (\( n = 0 \)). In other words, electrons are free to move in the \( xy \)-plane but not in the \( z \)-direction. In the AlGaAs/GaAs system, AlGaAs and GaAs have the same lattice constant, so there is no strain and hence few lattice dislocations and high electron mobility. To reduce scattering from the Si dopants, an undoped AlGaAs space layer is introduced between the GaAs and Si-doped AlGaAs layers. Electron mobility in this AlGaAs/GaAs heterostructure now reaches more than \( 3.5 \times 10^7 \text{ cm}^2\text{V}^{-1}\text{s}^{-1} \),\(^6\) and electron density can be controlled below \( 1 \times 10^{10} \text{ cm}^{-2} \).
1.1.2 Quantum wire and quantum dot

To reduce dimensionality further, low-dimensional nanostructures, such as quantum wires and quantum dots, are created. Two methods are often used to produce these nanostructures: ‘top-down’ and ‘bottom-up’. The ‘top-down’ method is to use lithography to pattern the nanostructures and etch away the material outside the patterns. However, it is not easy to control the etching process accurately down to nanoscale features. An alternative method is to use 2DEG systems and field-effect transistors. Nanoscale surface gates are patterned using lithographic techniques. When an electric field is applied, the electrons below the gates are depleted, forming nanostructures in the 2DEG. For example, a pair of split gates creates a thin 1D wire, and the conductance is quantised in units of $2e^2/h$.9–11 Similarly, the gate allows further confinement to be achieved and a quantum dot to be defined, as seen in Fig. 1.2 (a).12,13

The ‘bottom-up’ method is to self-assemble atoms and grow nanostructures on a substrate. By controlling the vapour or liquid sources, an axial heterostructure in nanowires or dots can also be created by epitaxial growth. We can also use lithographic techniques to position metal seed particles to control the position of the epitaxial growth of nanostructures,14 as shown in Fig. 1.2 (b). Nowadays nanowires and quantum dots are used in research, such as quantum information processing,15 single-photon sources,16 etc. Moreover, a surface acoustic wave, which includes a potential wave in piezoelectric materials, can couple to these nanostructures and allow more interesting physics to be discovered.

1.2 Surface acoustic waves

In nature, several modes of sound waves are defined based on different oscillations of the particles or atoms, as shown in Fig. 1.3. In general, these are classified into body
Chapter 1. Introduction and background

Figure 1.3: Different modes of a wave propagating on a solid substrate with different atom vibrations: (a) longitudinal wave (P-wave), (b) transverse wave (S-wave), (c) Rayleigh wave (SAW), and (d) plate wave with symmetric and asymmetric modes. All four modes of waves propagate from left to right, as the arrow shows.

waves and surface waves. In body waves, there are two main kinds: longitudinal and transverse (shear) waves. Longitudinal waves involve the particles oscillating in a longitudinal direction, or along the wave-propagation direction. Energy transfer is by a series of compression and expansion particle movements. Due to the longitudinal movement, particle density changes along the direction of wave propagation and these are also called density waves or pressure waves (P-waves). For shear waves (S-waves), the particle oscillates in a normal or transverse to the direction of propagation. Shear waves require a solid substrate for propagation, and are usually weaker than longitudinal waves. Longitudinal and shear waves are popular in ultrasonic inspection technology.

A surface (Rayleigh) wave travels along the surface of a thick solid substrate and only penetrates down to a distance of about a wavelength. These were discovered by Lord Rayleigh in 1885. The atoms oscillate in an elliptical orbit combining both longitudinal and transverse motion. Rayleigh waves are very sensitive to defects in the surface. Therefore the Rayleigh wave can be used to check surface roughness and also for mass sensing. Like surface Rayleigh waves, plate waves also combine the longitudinal and transverse motion of atoms, but they are only in a thin film (a few wavelengths thick). A Lamb wave is a wave propagating along the surface throughout the whole thickness of the substrate. There are two types of wave compressing and stretching the atoms. If the thin film is compressed and stretched in the wave propagation direction, this is called the symmetrical mode. If the
compression and stretching of the thin film are normal to the propagation direction, this is called the asymmetrical mode. More complicated, there is another plate wave with atoms oscillating parallel to the surface plane but perpendicular to the wave propagation direction. These are called Love waves (Q-waves). Table 1.1 summarises the different modes of sound waves and their atomic vibration direction.

Table 1.1: Sound waves propagating modes in a solid

<table>
<thead>
<tr>
<th>Wave types</th>
<th>Atom vibration</th>
</tr>
</thead>
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<tr>
<td>Body wave</td>
<td></td>
</tr>
<tr>
<td>P-wave</td>
<td>Longitudinal</td>
</tr>
<tr>
<td>S-wave</td>
<td>Transverse</td>
</tr>
<tr>
<td>Surface wave</td>
<td></td>
</tr>
<tr>
<td>Surface wave (Rayleigh)</td>
<td>Elliptical orbit</td>
</tr>
<tr>
<td>Plate waves</td>
<td></td>
</tr>
<tr>
<td>Lamb wave</td>
<td>Perpendicular to wave direction</td>
</tr>
<tr>
<td>Love waves</td>
<td>Parallel to surface</td>
</tr>
</tbody>
</table>

In this thesis, we focus on the Rayleigh waves or surface acoustic waves (SAWs). In an isotropic elastic material, the atoms oscillate in an elliptical orbit and induce strain in the lattice, causing mechanical waves to propagate along the surface at the speed of sound. In an anisotropic piezoelectric material, this deformation of the lattice or strain waves generates changes in charge polarization, creating electric fields, which is known as the piezoelectric effect. These electric fields also excite a change in strain as the sound wave propagates. Hence a SAW is a combination of a mechanical wave and an electric potential wave. The stress and the electric displacement in both non-piezoelectric and piezoelectric case are given by:

\[
\begin{align*}
T &= \begin{cases} 
C \cdot S & \text{Non-piezoelectric} \\
C \cdot S - \varepsilon^T \cdot E & \text{Piezoelectric}
\end{cases} \\
D &= \begin{cases} 
\varepsilon \varepsilon_0 E & \text{Non-piezoelectric} \\
e \cdot S + \varepsilon \cdot E & \text{Piezoelectric}
\end{cases}
\end{align*}
\tag{1.3, 1.4}
\]

where \( C \) is the elastic constant matrix, \( e \) is the piezoelectric constant matrix, \( \varepsilon \) is dielectric constant matrix, and \( S \) and \( E \) are the strain and electric field matrices.

In a cubic crystal, such as GaAs, the \( 6 \times 6 \) stress constant matrix is reduced to the three independent components due to high symmetry.

\[
C = \begin{bmatrix}
C_{11} & C_{12} & C_{12} & 0 & 0 & 0 \\
C_{12} & C_{11} & C_{12} & 0 & 0 & 0 \\
C_{12} & C_{12} & C_{11} & 0 & 0 & 0 \\
0 & 0 & 0 & C_{44} & 0 & 0 \\
0 & 0 & 0 & 0 & C_{44} & 0 \\
0 & 0 & 0 & 0 & 0 & C_{44}
\end{bmatrix}
\]

Similarly the piezoelectric and dielectric constant matrix becomes:

\[
e = \begin{bmatrix}
0 & 0 & 0 & e_{14} & 0 & 0 \\
0 & 0 & 0 & 0 & e_{14} & 0 \\
0 & 0 & 0 & 0 & 0 & e_{14}
\end{bmatrix}
\]
From the stress and displacement (Eqns. 1.3 and 1.4), the particle displacement, \( u_{ijkl} \), are given by Eqns. 1.5 and 1.6

\[
\rho \frac{\partial^2 u_j}{\partial t^2} = C_{ijkl} \frac{\partial^2 u_k}{\partial x_i \partial x_j} + \varepsilon_{ikl} \frac{\partial^2 \phi}{\partial x_i \partial x_l},
\]

(1.5)

\[
\varepsilon_{ik} \frac{\partial^2 \phi}{\partial x_i \partial x_l} = \varepsilon_{ikl} \frac{\partial^2 u_k}{\partial x_i \partial x_l},
\]

(1.6)

where \( \rho \) is the mass density of the substrate. To solve Eqn. 1.5, we use a trial solution:

\[
u = u_0 e^{-bkz} e^{ik(x-vt)},
\]

(1.7)

where \( b \) is constant and \( k \) is the wave number. To obtain the numerical solution of the partial differential equation, we need boundary conditions. Firstly, the stress component along the plane \( z = 0 \) is zero

\[
T_{xz} = T_{yz} = T_{zz} = 0.
\]

(1.8)

Secondly, following the continuous charge displacement at the interface, another boundary condition is given as:

\[
D_z(\text{air}) = D_z(\text{sub}).
\]

(1.9)

By solving the wave equation with boundary conditions (Eqns. 1.8 and 1.9), the atomic displacements and piezoelectric potential are calculated as a function of depth from the surface, as shown in Fig. 1.4. The particle displacement shows that the SAW only penetrates around one wavelength below the surface.

Figure 1.4: Particle displacement in \( x \) and \( z \) directions (left) and SAW potential (right) in a GaAs substrate.
In experiments, inter-digital transducers (IDTs) are used to generate and detect SAWs. On a piezoelectric substrate, a strip of thin metal fingers is deposited. A radio frequency (RF) signal at the SAW resonant frequency is applied to the half of the IDTs, with the other half grounded. The alternating electric fields excite the piezoelectric effect and SAWs are launched and propagate on the substrate. The propagating velocity of the SAW mainly depends on the properties of the substrate material, such as mass density, elastic constant etc. In anisotropic piezoelectric substrates, the different crystal orientations give different SAW propagation speeds. For example the SAW speed on a 128° Y-cut LiNbO$_3$ substrate is around 3990 ms$^{-1}$, and on a 64° Y-cut LiNbO$_3$ substrate, it is around 4742 ms$^{-1}$. Moreover, if the SAW propagates on a thin film, the velocity also depends on the thickness of the film. Table 1.2 shows the SAW velocity in different substrates.

<table>
<thead>
<tr>
<th>Substrate</th>
<th>Crystal cut</th>
<th>Propagation axis</th>
<th>Velocity (m/s)</th>
<th>$K^2$ (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Quartz</td>
<td>ST</td>
<td>X</td>
<td>3158</td>
<td>0.11</td>
</tr>
<tr>
<td>LiNbO$_3$</td>
<td>Y</td>
<td>Z</td>
<td>3488</td>
<td>4.5</td>
</tr>
<tr>
<td>LiNbO$_3$</td>
<td>128°</td>
<td>X</td>
<td>3992</td>
<td>5.3</td>
</tr>
<tr>
<td>GaAs</td>
<td>&lt;001&gt;</td>
<td>&lt;110&gt;</td>
<td>∼2800</td>
<td>0.06</td>
</tr>
<tr>
<td>ZnO</td>
<td>&lt;001&gt;</td>
<td>&lt;100&gt;</td>
<td>∼2600</td>
<td>1.15</td>
</tr>
</tbody>
</table>

Table 1.2: SAW properties for different piezoelectric substrates.

To detect SAWs, another set of IDTs is deposited on the other side of the substrate as a receiver. We use an electromechanical coupling coefficient $K^2 = \frac{e^2}{c\varepsilon}$ to characterise the conversion between electrical energy and mechanical energy, where $e$ is the piezoelectric coefficient, $c$ is the elastic constant and $\varepsilon$ is the dielectric constant. Experimentally, $K^2$ is measured by the relation $K^2 = \frac{2\Delta v}{v}$, where $\Delta v$ is the change in SAW velocity when the SAW path is shorted by a metal sheet on the surface. The higher coupling coefficient means more efficient conversion between the electrical energy and mechanical energy. This coefficient is a very important parameter when choosing the substrate for SAW application. Table 1.2 gives the SAW velocity and coupling coefficient for different substrates. Among these, LiNbO$_3$ is the most popular piezoelectric substrate because of its high coupling coefficient (5%).

The period of IDTs determines the SAW wavelength and therefore the resonant frequency. Figure 1.5(a) depicts a single finger IDT design. The SAW wavelength is equal to the period of the transducer fingers. Given a metallisation ratio of 0.5, the width of metal fingers and the separation between fingers are both a quarter of the wavelength. The overlap length of fingers determines the SAW beam width, and the SAW resonance bandwidth decreases as the number of finger pairs increases. Furthermore, other IDT designs that meet different requirements for SAW applications. Fig. 1.5(b) demonstrates split fingers to reduce the reflection of SAWs from each finger by choosing the right phase shift between two fingers. The bandwidth is larger as there are no multiple reflections under the IDT, but the emitted SAW amplitude is lower. Usually, the IDTs generate SAWs in two directions, and 50% of power is wasted in generating the SAWs going in the unwanted direction. By adjusting the phase shifts of fingers, the bidirectional SAW is modified to a unidirectional SAW.
Chapter 1. Introduction and background

Figure 1.5: Inter-digital transducer designs. (a) Single finger IDT with a wavelength of $\lambda$ (equal to the finger period) and beam width $W$ (finger overlap length). (b)-(d) Different IDT designs, including double (split-finger) IDT, fin IDT and unidirectional IDT. (e) Equivalent circuit of SAW IDTs.
by a special transducer architecture (Fig. 1.5(d)). Fig. 1.5(c) shows the Fin IDTs structure designed to excite SAW over a large bandwidth and even used to map the position across the IDT to different resonant frequencies.

Figure 1.5(e) shows the equivalent circuit of IDTs, with the metal fingers working as a set of capacitors in parallel, \( C_T(f) = NWC_0(f) \), where \( N \) is the number of IDT finger pairs, \( W \) is the finger overlap length, and \( C_0(f) \) is the capacitance per unit length. Due to electromagnetic radiation, radiation susceptance \( (B_a(f)) \), the imaginary part of admittance) and conductance \( (G_a(f)) \), the real part of admittance) factors are also introduced into the equivalent circuit. From the impulse response model, the radiation conductance and susceptance are expressed by:

\[
G_a(f) = 8K^2NC_0f_0N^2\frac{\sin(X)}{|X|}^2
\]

\[
B_a(f) = \frac{8N^2G_0\sin(2X) - 2X}{2X^2},
\]

where \( K^2 \) is the electromechanical coupling coefficient, \( G_0 \) is the electrical characteristic admittance of the equivalent SAW transmission line \( G_0 = K^2C_Tf_0 \), \( X = N\pi(f - f_0)/f_0 \) and \( f_0 \) is the centre resonant frequency. \( B_a(f) \) relates to energy storage in the strain field with SAW excitation, and goes to zero at the centre frequency. Usually it is omitted in calculations.\(^{18}\)

To obtain the maximum power transfer into an IDT, we match the load impedance to the source impedance, usually 50Ω. For high-frequency SAWs, an impedance-matching circuit is essential.

Figure 1.6: Stroboscopic photoluminescence spectrum in a single AlGaAs/GaAs quantum dot with different SAW waveforms (a,e) sine waves, (b,f) square waves, (c,g) sawtooth waves, (d,h) \( \delta \)-shape waves. Figures from Ref. 19.

By varying the period of IDTs, the SAW resonant frequency is tuned from the MHz to the GHz range level. For MHz-1 GHz SAWs, standard optical lithography can be utilised to pattern fingers down to a few micrometres. However, for SAWs of a higher frequency (a few GHz), electron-beam lithography is used to pattern IDT
fingers on a sub-micron scale. Even with high-resolution electron-beam lithography, the finger width and separation are still difficult below to 100 nm feature sizes. This is because there are tens of hundreds of pairs of thin fingers in an IDT. For mass production, Van Der Wiel’s group has developed a nano-imprint stamp to print the IDT fingers, instead of electron-beam lithography, down to 65 nm,\textsuperscript{20} which may make the mass-production of such IDTs quite cheap. To obtain an ultra-high frequency SAW, we can also use higher harmonic modes of the fundamental Rayleigh mode. The 7\textsuperscript{th} harmonic mode of a Rayleigh wave has reached a frequency of 23 GHz.\textsuperscript{20} However, the low quality factor and small bandwidth make it challenging to use in a high-frequency SAW filter. More interestingly, Krenner \textit{et al.} have developed a technique to generate different SAW waveforms with the help of high harmonic modes. Figure 1.6 shows different SAW waveforms, such as a sine wave, a square wave, a sawtooth wave, and a $\delta$-shape wave.\textsuperscript{19}

\section*{1.3 Review of SAW researches}

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure1.7.png}
\caption{An example of acoustoelectric current plateaus. The power applied to the transducer is varied from 13 dBm to $-5$ dBm in steps of 0.02 dBm. Inset: schematic diagram of SAW devices. Figure from Ref. 21,22.}
\end{figure}

Nowadays the SAW technique is used extensively for signal processing in televisions, mobile phones, radar and others. SAWs propagate at the speed of sound (3000 m/s), which is five orders of magnitude smaller than an electromagnetic wave ($3 \times 10^8$ m/s). It is possible to design a MHz-GHz SAW delay-line filter in a millimetre-size chip, which is much easier in terms of architecture and manufacture than an electromagnetic wave filter. Every day there are around 1 million SAW filters and duplexers produced and used in the signal communications industry. Apart from the commercial use of SAW filters, there are some other applications of SAWs,
such as sensors. A SAW propagating on the surface of a piezoelectric substrate is very sensitive to mass loading on the surface. SAW (or other modes of waves) delay lines are designed as mass sensors for gases and liquids, and as biosensors. In chemistry, SAW can excite a certain catalyst and hasten the chemical reaction. Meanwhile, SAWs also stimulate an interest in quantum physics, which is preparing for next-generation technology.

### 1.3.1 SAWs in nanoelectronics

When a SAW propagates in a GaAs/AlGaAs heterostructure with two-dimensional electron gas, electrons are trapped in the SAW potential minima, moving in the SAW propagation direction. When sweeping the voltage on split gates on either side of the channel, and the transverse confinement becomes strong, forming a dynamic quantum dot in each SAW minimum in the region below the gap between gates. As the gate voltage becomes further negative, the number of electrons in each dot decreases and we can observe quantised current $I = Nef$ where $N$ is the number of electrons in each minimum and $f$ is the SAW resonant frequency, as shown in Fig. 1.7. Experimentally, in 1996 Shilton et al. demonstrated quantised SAW-driven current with the first two plateaux ($I = ef$ and $I = 2ef$) through a split-gate-defined quasi-one-dimensional (1D) channel. Consequently, a clear quantised current with high accuracy of 60 parts per million was observed. This SAW-driven quantised current offers new possibilities in metrological applications for current standards.

For metrological applications to redefine Ampere, accuracy should be better than one hundred parts per billion. However, the flatness of SAW plateaus was never sufficient. To study the electron dynamics in a SAW and the error mechanisms, Quantum tunnelling was considered as the main error mechanism. To investigate electron oscillation and tunnelling in SAW dynamic quantum dots, Astley
and Kataoka designed a dual-SAW-channel device, which contained two independent SAW channels in an “X” junction, as seen in Fig. 1.8 (a). The two SAW channels were separated by a narrow tunable tunnel barrier and surrounded by six gates to control the tunnel-barrier height and the width of each channel. The SAW-driven current was quantised at $1e_f$, $2e_f$ and $3e_f$. By controlling the barrier, there was a small current tunnel through the barrier and there was a small deviation from the input current to the output current. In the experiment, small oscillations were seen in the tunnelling current. Figure 1.8(b) demonstrates the coherent oscillation in the wave-function of an electron in a dot between two channels. This phenomenon indicates that electrons in SAW quantum dots may tunnel through the barrier to the other SAW channel, and the tunnelling rate was dependent on the barrier potential and the dot occupancy.

In 2007, Kataoka et al. achieved the single-electron population and depopulation of an isolated static quantum dot with a pulse of SAWs. A static quantum dot is defined by surface gates. Once one electron occupies the dot, the Coulomb blockade prevents another electron populating to this dot. When a SAW passes through the dot, the electron tunnelling probability is enhanced. A pulse of SAWs thousands of periods is long enough that a single electron in the dot ensures tunnels out. Therefore, it is possible to control the single electron population and depopulation in an isolated quantum dot with SAWs. Hermelin et al. demonstrated a high-efficient single-electron transfer in 2011. In Fig. 1.9(a), with SAWs a single electron is transported from one dot to another dot through a 1D channel as a high quantum efficiency emission and detection of 96% and 92% respectively. At same time McNeil et al. successfully achieved repeatable single-electron transfer between two distant quantum dots, as seen in Fig. 1.9 (b) and (c). Two quantum dots are created by surface gates, connected by a 4 $\mu$m channel. Two split-finger IDTs are placed to generate SAW pulse in opposite directions. When a pulse of SAWs is applied from the left, an electron is depopulated from the left dot, travelling 4 $\mu$m, and populates the right empty dot. A pulse of SAWs is then applied from the right, and the electron leaves the right dot and arrives back in the left dot. This Ping-Pong-like transport shows that the electrons can be transferred between two quantum dots 60 times, travelling 250 $\mu$m without errors.

### 1.3.2 SAWs in quantum optics

SAWs have shown a strong ability to manipulate single electrons. If SAWs also control or transport electrons and holes, they can be utilised in quantum optics. Rocke et al. have found that an electron-hole pair, excited by a laser beam, can be stored in SAWs (electrons in minima and holes in maxima) over orders of magnitudes longer than the recombination lifetime. In other words, with the help of SAWs, the radiative lifetime can be prolonged by orders of magnitude. According, Couto et al. and Hernández-Mínguez et al. successfully demonstrated the photon anti-bunching with SAWs in 2009 and 2011 respectively, as shown in Fig. 1.10 (a-d). Couto et al. used a laser to generate electron-hole pairs, and SAWs to separate and transport electrons and holes. The electrons and holes were then captured and recombined in a quantum wire embedded in a GaAs quantum well (as seen in Fig. 1.10(c)). Similarly, A. Hernández-Mínguez et al. used GaAs-based nanowires
Section 1.3. Review of SAW researches

Figure 1.9: Electron micrograph of the dot-channel-dot SAW device in Hermelin’s (a) and McNeil’s works (b). (c) Dot conductance as a function of time. At time A the channels are initialised to be empty. Between times A and B, a series of control pulses is used to verify that the system is still empty. At time B an electron is loaded into the left quantum dot (LQD). Between times B and C, there is a two-way transfer of a single electron between the quantum dots. At time C, the electron is removed from the system using a clearing pulse. Figure from Ref. 30,31.
Figure 1.10: (a) Schematic diagram of a GaAs nanowire on a LiNbO$_3$ substrate with transducers. Inset: SAW-modulated band edge with carrier recombination at different positions on the nanowire. (b) Photon correlation histograms with an antibunching effect at a zero time delay. Figures from Ref. 33. (c) Schematic diagram of an acoustically pumped photon source. A laser beam excites the electron-hole pairs and SAWs drag them to the short quantum wires (triangles), where electrons and holes recombine and generate photons. (d) Photon correlation histograms with antibunching effect at different powers. Figures from Ref. 34. (e) Schematic diagram of a lateral $n$-$p$ junction in a [100]-[311]A-[100] step. IDTs generate SAWs at [100] surface. (f) Luminescence spectrum as a function of frequency and wavelength. The luminescence peak shows at the SAW resonant frequency with photo energy matching the band gap of the GaAs quantum well. Figures from Ref. 35.
Section 1.3. Review of SAW researches

on a LiNbO$_3$ substrate, as seen in Fig. 1.10(a). Figures 1.10(b) and (d) describe photoluminescence measurements and correlation data analysis. The missing peak at a zero time delay in correlation data indicates photon anti-bunching. As in quantum wells and quantum wires, the SAW-driven photon anti-bunching is also observed in GaAs/AlGaAs micro-pillar cavities. A single-photon source with a high repetition rate will be essential for quantum information processing, such as quantum key distribution and quantum repeaters.

The above works on SAW-driven single-photon sources are based on photoluminescence (PL) with a laser beam to excitons (electron-hole pairs), which are hard to control and manipulate electrically as they are neutral. Using SAW single-electron pumping, a new idea to achieve a single electron source and detection was proposed by Foden et al. involving an electrocluminescence (EL)-based single-photon source, based on SAWs and an $n$-$p$ junction. When a stream of single electrons in each SAW minimum enters an area with free holes, electrons recombine with holes and generate a stream of single photons. To realise a SAW-driven single-photon source in an $n$-$p$ junction experimentally, a lot of research has been undertaken. Figure 1.10 (e) demonstrates a lateral $n$-$p$ junction by modulation doping techniques on a GaAs/AlGaAs wafer. The electrical luminescence measurement showed the success of photon generation from SAW-driven electrons and holes (as seen in Fig. 1.10 (e)). Meanwhile, similar luminescence measurements have been carried out by Simoni et al. on an induced $n$-$p$ junction.

More recently, Hsiao et al. have observed photon anti-bunching in an undoped GaAs heterostructure. Free electrons and holes are induced by external electric fields forming a lateral $n$-$p$ junction. The SAW pumping current is at or below $ef$, where $f$ is the SAW resonant frequency, so that a stream of single electrons is dragged by SAWs and recombines with holes. The apparent dip at zero time delay in the correlation measurement indicates photon anti-bunching. However, $g^{(2)}(0)$ is just below 0.5, which may be because of the absence of the SAW quantisation. Further improvements in the quantum confinement of SAW-driven quantum dots is important.

### 1.3.3 SAWs in spintronics

In spintronics, the strong exchange interaction between electron spin and hole spin is a big challenge in manipulation and transportation of the spin. If a SAW can delay electron-hole recombination, it may also extend the spin lifetime. To experimentally prove the assumption, in 2001 Sogawa et al. demonstrated an improvement in the transport and lifetime of photo-excited electron and hole spins with SAWs in a GaAs quantum well. The polarisation of the photon determines the initial spin, and the output spin was read from the polarisation of recombined electron-hole pairs. The electrons and holes separate SAW minima and maxima, and the strong exchange interaction between spins was suppressed. The results showed that spin states could be transported over 3 $\mu$m and the spin relaxation times were two orders of magnitude longer than those without SAW modulation. Further works by Stotz et al. showed that coherent spin transport could exceed 100 $\mu$m in a GaAs quantum well. Figure 1.11(a) demonstrates this work. A pair of perpendicular transducers was placed on the substrate and generated two beams of coherent acoustic phonons.
Figure 1.11: (a) Schematic view of an array of dynamic quantum dots (DQDs) created by the interference of two beams of coherent acoustic phonons (CAPs) along [110] and [1\(\bar{T}0\)] directions and a photoluminescence density of the DQDs. Figure from Ref. 45. (b) Schematic diagram of the device on a wafer with a GaAs quantum well. A SAW is launched by IDT and propagated on a thin film with slits that creates straight or winding channels. Figure from Ref. 46. (c) Scanning electron microscope image of spin-transfer dot-to-dot devices. Two quantum dots are defined by surface gates separated by a long channel. A SAW is launched by transducers on the left. The static dots are used to initialise and detect electron spin. Figure from Ref. 47.
(CAPs) along the [110] and [1$ar{1}$0] direction, respectively. When the two CAPs overlapped in a particular region, an array of dynamic quantum dots was formed, confining the particle’s movement in all three dimensions. As before, the polarised photon emission was observed and demonstrate the polarised excitation.

In quantum information processing, electron spin resonance (ESR) is generally used to manipulate electron spins. Sogawa’s group developed a magnetic-field-free ESR using a strong spin-orbit effect with a SAW along a winding semiconductor channel,\(^{46}\) as shown in Fig. 1.11(b). Furthermore, in continuing work on the single electron transfer between distant quantum dots, Bertrand et al. have demonstrated the long-distance electron spin transfer between distant quantum dots, as shown in Fig. 1.11(c). They initialise the spin of a single electron using the Zeeman energy, and the Pauli principle for two electrons in a quantum dot. A pulse of SAWs then moves the electrons to another quantum dots a few micrometres away. They observed a long distance spin transfer with a fidelity of 65%. This transfer may realise a transfer of the qubit over a few microns between static qubits.\(^{47}\) This research, based on SAWs, may pave the way towards quantum spintronics and quantum information processing.

### 1.3.4 SAWs in magnetoacoustics

A SAW introduces a strain wave along the surface of a substrate. In magnetic materials, spin waves, as propagating spin disturbances, are equivalent to quasiparticles, called magnons. SAWs can couple to spin waves and therefore control the magnetisation resonance in a ferromagnetic thin film, which is termed as magnetoacoustics. Weiler et al. demonstrate elastically driven ferromagnetic resonance in a thin Ni film on a LiNbO$_3$ substrate (as seen in Fig. 1.12(a)).\(^{49}\) At room temperature, they compared the insertion loss $S_{12}$ at different external magnetic fields at a certain angle. At the fundamental Rayleigh mode at 0.17 GHz, the SAW cannot excite the magnon. As it utilises the high-harmonic mode, the SAW succeeds in exciting the ferromagnetic resonances. Weiler et al. have also demonstrated SAW-driven spin current by coupling phonons to magnons in a Co/Pt layer, as seen in Fig. 1.12(b).\(^{50}\) This work offers an approach to testing the magnon-phonon interaction with SAWs. Later Thevenard et al. demonstrated the precessional magnetisation switching using a SAW on a (Ga, Mn)(As,P) thin film.\(^{52}\) In 2017 Foerster et al. developed a new technique for simultaneous imaging of SAW-induced magnetisation on a nanometer scale, as shown in Fig. 1.12(c). A SAW pulse excites the magnetisation of Ni squares on the LiNbO$_3$ substrate, and then changes in the domain wall can be imaged using stroboscopic X-ray microscopy.\(^{51}\)

### 1.3.5 SAWs in qubits

In quantum information technology, circuit quantum electrodynamics (QED) is popular in the investigation of the physical interaction between the photons and quantum atoms, here usually referred to as artificial atoms or qubits, which can be used for quantum computing.\(^{54,55}\) In the quantum regime, $\hbar \omega >> k_B T$, a high resonant frequency of 5–10 GHz is needed for coupling to a transmon qubit. In the case of SAWs, it is an advantage to match the resonant frequency for the transmon qubits
Figure 1.12: (a) Schematic diagram of a device for ferromagnetic resonance. IDTs are deposited on the LiNbO$_3$ substrate with a nickel film on the surface. The closeup shows the strain $\varepsilon$ in the Ni film. Figure from Ref. 49. (b) Instead of Nickel film, a Co/Pt film is present on the surface of the LiNbO$_3$ substrate. The closeup shows the SAW-driven magnetisation $M$ emitting a spin current $J_S$ into a Pt film measured by inverse spin Hall effect $E_{ISH}$. Figure from Ref. 50. (c) Schematic diagram of the device for magnetisation imaging. X-rays illuminate the sample in the form of pulses at 500 MHz. IDT1 generates a piezoelectric SAW at around 500 MHz propagating through the LiNbO$_3$ substrate and interacting with the magnetic nanostructures. The variation in the piezoelectric voltage on the surface sample is probed with photoemission electron microscopy (PEEM), as is the magnetisation contrast along the X-ray propagation direction arising from the X-ray magnetic circular dichroism (XMCD) effect. In an XMCD image of the same structures, magnetic domains are shown within the Ni squares. Figure from Ref. 51.
Section 1.3. Review of SAW researches

Figure 1.13: A: Electron micrograph of the device with SAW IDTs and a QED qubit. B: The equivalent circuit of the SAW-coupled qubit. $C_{tr}$ is the geometric capacitance of the finger structure. It is shunted by a SQUID, which acts as a nonlinear inductance $L_J$ that can be adjusted with a magnetic flux $\Phi$. $Y_{a,tr}$ is the acoustic admittance element that can pick up a SAW from the IDT (red arrow) to produce electrical excitation in the qubit and regenerate it as a SAW with a phase shift (blue arrow). An RF voltage is also applied to the $C_{gate}$ to manipulate the qubit. C: The reflection $|\Delta S_{11}|$ as a function of qubit magnetic flux $\Phi/\Phi_0$. Manipulating the qubit with a gate and receiving the quantised phonons, up to three, in the experiment (D), and model (E). Figures from Ref. 53.
to phonon. Therefore, it is possible to build the QED to investigate the physical interaction between the artificial atoms and phonons, rather than photons. In 2014 Per Delsing’s group demonstrated single 5 GHz SAW phonons interacting with an artificial atom in a regime of strong coupling, as shown in Fig. 1.13. The IDTs, matching the resonant frequency of a transmon, worked as a phonon emitter and receiver. By tuning magnetic flux $\Phi$ through a superconducting quantum interference device (SQUID), the qubit resonance matched the SAW and increased the SAW reflection, indicating the emitted phonons. By increasing the gate RF power, more phonons were emitted, as seen in Fig. 1.13(d). These results show that it is possible to create a design involving two semiconductor qubits coupled by a SAW. Later P. Leek’s group demonstrated a transmon qubit with IDTs in the SAW resonator cavity. This experiment is another example of superconducting qubit coupling to SAWs. Moreover, Barnes et al. proposed the idea of implementing qubits with SAW-driven quantum dots. In two crossing SAW-channels, by controlling the electron spin in SAW-driven dynamic quantum dots with nanomagnets to carry out quantum computing. However, this proposed SAW qubit has not been realised.

The above research has shown that a SAW can couple to nanostructures and allow interesting quantum phenomena to be observed. In this dissertation, we investigate the SAW couples to GaAs and ZnO heterostructures, and focus on the low-dimensional electron transport.

1.4 Layout of the thesis

Chapter 1 introduces the low-dimensional electron transport in nanostructures, as well as the mechanism of surface acoustic waves and their applications in quantum physics.

Chapter 2 discusses the simulation of gate-patterned quantum devices in both doped and undoped GaAs heterostructures, emphasising the importance of boundary conditions.

Chapter 3 describes the fabrication and measurement of a SAW spectroscopy device. It also explains error mechanisms of SAW quantisation in a magnetic field.

Chapter 4 describes the success of ZnO sputtering on a GaAs/AlGaAs heterostructure. It shows the enhancement of SAW pumping with the help of the ZnO overlayer.

Chapter 5 introduces a MgZnO/ZnO heterostructure and discusses the fabrication of a quantum wire using quantum point contacts and the result of the one-dimensional ballistic electron transport and the prominent N.7 structures.

Chapter 6 describes the theoretical and experimental investigation of the SAW modulation on the MgZnO/ZnO heterostructure.

Chapter 7 concludes what we have achieved and what could be achieved in future.
Simulations of gate-patterned quantum devices

Gate-patterned devices using a two-dimensional electron gas (2DEG) allow the investigation of a variety of effects, such as ballistic electron transport,\textsuperscript{9,58,59} Coulomb blockade,\textsuperscript{60,61} and spin read-out\textsuperscript{7,13} and they are also being developed for quantum computation.\textsuperscript{62} To understand the potential of such devices, and to optimise their designs, it is essential to calculate their electrostatic potential distribution with specific patterned gates and various biases. However, the most realistic surface and back boundary conditions (BCs) are still controversial despite much work over the years.\textsuperscript{63–71} In this work we calculate three-dimensional electrostatic potentials using a standard commercial partial differential equation (PDE) solver package, Nextnano.\textsuperscript{72} We compare simulations with a range of experimental verifications, with doped and undoped GaAs-based heterostructures, and patterned-gate structures with and without a surface dielectric layer. We find that the models match experiments much more closely, and have a much greater predictive power in device architectures if one chooses the BCs carefully.

This part of the work on induced lateral \textit{n-i-n} and \textit{n-i-p} junctions, including device fabrication, measurements and modelling involved the collaboration of Dr. Yousun Chung and Dr. Tzukan Hsiao.

2.1 Finite-element method and Thomas-Fermi model

In the numerical analysis, the finite-element method (FEM) is popular for solving complicated physics problems. By dividing an entire domain into finite elements, PDE is solved in each small element and then assembled over the whole domain. In each element, we seek an approximate solution $\tilde{u}$, compared to the exact solution $u$ in a linear combination of mesh-dependent basis functions $\{\phi_1, \phi_2, \ldots, \phi_N\}$,

$$\tilde{u} = \sum_{i=1}^{N} u_i \phi_i,$$

(2.1)

where $N$ is the number of nodes in each element. To solve the PDE, it is only necessary to find the coefficients $u_i$ to fit solution $\tilde{u}$ closest to $u$. 

21
Chapter 2. Simulations of gate-patterned quantum devices

Figure 2.1: Finite-element meshes of a semiconductor device frame.

\[ \tilde{u} - u = 0. \] (2.2)

To achieve this, the weight residual method and the weak formulation are applied,

\[ \int_{\Omega} RW_i d\Omega = 0, \quad i = 1, 2, \ldots, N, \] (2.3)

where the residual \( R = D(\tilde{u}) \), \( D \) is a differential operator, and \( W_i \) is the weighting function. In the weak formulation, \( W_i \) is set to be the basis function \( \phi_i \), and \( \Omega \) is the arbitrary domain. FEM is then applied to the electrostatic Poisson equation:

\[ \nabla^2 \phi(\mathbf{r}) = -\frac{\rho(\mathbf{r})}{\varepsilon_0 \varepsilon(\mathbf{r})} \] (2.4)

where \( \rho(\mathbf{r}) \) is the carrier density, and \( \varepsilon_0 \) and \( \varepsilon(\mathbf{r}) \) are the relative permittivity for vacuum and dielectric constants of semiconductors. Here Eqn. 2.4 is simplified:

\[ -\nabla^2 u = f, \] (2.5)

\[ -\frac{\partial}{\partial x}(\frac{\partial u}{\partial x}) - \frac{\partial}{\partial y}(\frac{\partial u}{\partial y}) - \frac{\partial}{\partial z}(\frac{\partial u}{\partial z}) = f. \] (2.6)

There are two types of boundary conditions: the Neumann boundary condition is given by:

\[ \frac{\partial u}{\partial x} + \frac{\partial u}{\partial y} + \frac{\partial u}{\partial z} = A, \] (2.7)

and the Dirichlet boundary condition is defined by:

\[ u(x,y,z) = B, \] (2.8)

where \( A \) and \( B \) are known functions or constants on the boundary. Here Poisson equation is inserted into the weighted residual, and Eqn. 2.3 becomes

\[ \int_{\Omega} \phi_i \left[ \frac{\partial}{\partial x}(\frac{\partial \tilde{u}}{\partial x}) + \frac{\partial}{\partial y}(\frac{\partial \tilde{u}}{\partial y}) + \frac{\partial}{\partial z}(\frac{\partial \tilde{u}}{\partial z}) \right] d\Omega + \int_{\Omega} \phi_i f d\Omega = 0. \] (2.9)

With Green’s formula (Eqn. 2.10):

\[ -\int_V (\phi \nabla^2 u + \nabla u \cdot \nabla \phi) d^3x = \oint_S \phi \frac{\partial u}{\partial n} da, \] (2.10)
Eqn. 2.9 becomes
\[
- \int_{\Omega} \left( \frac{\partial \tilde{u}}{\partial x} \left( \frac{\partial \phi_i}{\partial x} \right) + \frac{\partial \tilde{u}}{\partial y} \left( \frac{\partial \phi_i}{\partial y} \right) + \frac{\partial \tilde{u}}{\partial z} \left( \frac{\partial \phi_i}{\partial z} \right) \right) d\Omega - \int_{\partial \Omega} \phi_i \frac{\partial \tilde{u}}{\partial n} d\Gamma + \int_{\Omega} f d\Omega = 0,
\]
(2.11)

where \( \Gamma = \partial \Omega \). Then \( \tilde{u} \) is substituted for Eqn. 2.1, and the integral is transferred to a matrix form
\[
- \int_{\Omega} \left( \frac{\partial \phi_i}{\partial x} \frac{\partial \phi_j}{\partial x} u_j + \frac{\partial \phi_i}{\partial y} \frac{\partial \phi_j}{\partial y} u_j + \frac{\partial \phi_i}{\partial z} \frac{\partial \phi_j}{\partial z} u_j \right) d\Omega - \int_{\partial \Omega} \phi_i \frac{\partial u_j \phi_j}{\partial n} d\Gamma + \int_{\Omega} \phi_i f d\Omega = 0,
\]
(2.12)

\[MU = F,\]
(2.13)

where \( M \) is the ‘stiffness’ matrix given by
\[
M = \int_{\Omega} \nabla \phi_i \cdot \nabla \phi_j d\Omega = \sum_E M^E_{ij},
\]
(2.14)

and \( M^E_{ij} \) is a stiffness matrix of an element. \( F \) is given by:
\[
F_{ij} = \int_{\partial \Omega} \phi_i \frac{\partial u_j \phi_j}{\partial n} d\Gamma - \int_{\Omega} \phi_i f d\Omega.
\]
(2.15)

Then the integral is then evaluated through a mapping \( f_E : \hat{E} \rightarrow E \), where \( \hat{E} \) is the reference element
\[
M^E_{ij} = \int_{\hat{E}} \nabla \phi_i \cdot \nabla \phi_j |J_E| d\hat{\Omega},
\]
(2.16)

where \( |J_E| \) is the determinant of a Jacobian matrix of \( f_E \). In the transformation of the basis, the Jacobian is derived from:
\[
\begin{bmatrix}
\frac{\partial \phi_1}{\partial x} \\
\frac{\partial \phi_1}{\partial y} \\
\frac{\partial \phi_1}{\partial z}
\end{bmatrix}
= J^{-1}
\begin{bmatrix}
\frac{\partial \phi_1}{\partial \xi_1} \\
\frac{\partial \phi_1}{\partial \xi_2} \\
\frac{\partial \phi_1}{\partial \xi_3}
\end{bmatrix},
\]
(2.17)

so it becomes
\[
J =
\begin{bmatrix}
\frac{\partial x}{\partial \xi_1} & \frac{\partial y}{\partial \xi_1} & \frac{\partial z}{\partial \xi_1} \\
\frac{\partial x}{\partial \xi_2} & \frac{\partial y}{\partial \xi_2} & \frac{\partial z}{\partial \xi_2} \\
\frac{\partial x}{\partial \xi_3} & \frac{\partial y}{\partial \xi_3} & \frac{\partial z}{\partial \xi_3}
\end{bmatrix}
\]
(2.18)

In this model, \( f_E \) is a map from a 3D tetrahedron into actual elements. Then the integral is then calculated numerically with Gaussian quadratures:
\[
M^E_{ij} = \sum_{k=1}^{K} \nabla \phi_i(\xi_k) \cdot \nabla \phi_j(\xi_k) w_k |J_E(\xi_k)|,
\]
(2.19)

where \( \xi_k \) refers to the integration points, \( w_k \) is the integration weight, and \( K \) is the number of sampling points. Finally, with boundary conditions, the calculation of matrices and vectors loops over all the elements and is assembled over the global domain. Figure 2.1 demonstrates an example of a semiconductor device divided into many elements from one-dimensional meshes to three-dimensional meshes.
Once the electrostatic potential $\phi(\mathbf{r})$ is solved using the electrostatic Poisson equation with finite-element analysis and given appropriate boundary conditions, we deduce the electron density $\rho(\mathbf{r})$ in the quantum system with Fermi-Dirac distribution and density of states $g_{2D}$:

$$f(E) = \frac{1}{e^{(E-E_F)/kT} + 1}$$  \hspace{1cm} (2.20)

$$g_{2D} = \frac{m^*}{\pi \hbar^2}$$  \hspace{1cm} (2.21)

$$n(\mathbf{r}) = \int_{E_C}^{E_F} \frac{g_{2D}}{\pi \hbar^2} f(E)dE,$$  \hspace{1cm} (2.22)

where $k$ is the Boltzmann constant, and $T$ is temperature. In Eqn. 2.21, $m^*$ is the effective mass of electron 0.067 $m_e$ in GaAs, and $m_e$ is the bare electron mass.

At beginning of the calculation, the potential is initialised. From the potential, we solve the charge density by an integral to the production of Fermi-Dirac distribution (Eqn. 2.20) and density of states (Eqn. 2.21) from the edge of the conduction band $E_C$ to the Fermi energy, $E_F$. Then from the charge density, the electrostatic potential is recalculated from Poisson equation. Then a weighting factor $\alpha$ is introduced on the new calculated potential, $\phi_2$, to the previous potential, $\phi_1$:

$$\phi_1 = (1 - \alpha)\phi_1 + \alpha\phi_2,$$  \hspace{1cm} (2.23)

where $0 < \alpha \leq 1$. Then a self-consistent process is executed until convergence with a fixed tolerance is achieved:

$$|\phi_1 - \phi_2| = \eta,$$  \hspace{1cm} (2.24)

where $\eta$ is the tolerance set by the user. In 3D calculation using Nextnano, we use the tolerance and residual to be $1 \times 10^{-4}$.

### 2.2 Boundary conditions

In solving Poisson equation $\nabla \cdot (\varepsilon \varepsilon_0 \nabla \phi) = -\rho$, one must specify, at the boundary, either the electrostatic potential $\phi$ (Dirichlet BCs) or its normal derivative $\partial \phi / \partial n$ (Neumann BCs), or a mixture of the two. For GaAs, the high density of surface-charge states pins the Fermi level at the surface near the middle of the band gap, $\sim 0.75$ eV below the conduction band minimum. At high temperatures, the charge is mobile and there is no difference between a gated surface and an exposed surface. At cryogenic temperatures, the surface charge does not vary as gate biases are changed i.e. it is ‘frozen’, because the temperature is too low (below 100 K) for charge to move out of traps in the donor layer or at the surface. If this were not the case, then split-gate devices would exhibit hysteresis or pinch off gradually over time, as the charge hops between surface states. This is not observed for 2DEGs, although for hole gases, charges may move between acceptors because it is less tightly bound.

Thus, if surface gates are varied while the device is cold, the exposed surface will no longer be an equipotential, although this is still a popular approximation as it simplifies the calculation. Chen et al. have considered similar surface BCs previously, and devised a sophisticated scheme to include the ‘air’ above the
surface. They have shown that Neumann BCs on the surface matched the full calculation with an air well, and give much better results than when using Dirichlet BCs. However, they did not consider the case of a surface dielectric instead of air. Here, we find that this layer causes a significant shift in the pinch-off voltage. We also apply the idea of frozen charge below the 2DEG, which is ignored in the above studies. There are interface states at the ‘dirty’ regrowth interface between the substrate and the heterostructure grown by molecular-beam epitaxy (MBE), which can be calculated from the built-in electric field arising from intentional and utentional dopants. These charge states are also frozen out, so this interface is no longer at a constant potential. Therefore, instead of using Dirichlet BCs at the regrowth interface, as is often done, we take a fictitious boundary significantly below the regrowth interface.

2.3 One-dimensional simulation

We start from one-dimensional (1D) simulation of GaAs/AlGaAs heterostructures. A GaAs/AlGaAs heterostructure consists of GaAs and Al$_x$Ga$_{1-x}$As layers with different thickness and Al content. Here we set the Al content at $x = 0.32$. To engineer semiconductor band structures, a common method is to use intentional modulation with Si atoms, leading to strong internal electric fields. Alternatively, a metallic surface gate provides external electric fields to bend the band structure. Figure 2.2(I) demonstrates two GaAs-based heterostructures. The first structure is a GaAs high-electron-mobility-transistor (HEMT) heterostructure, which consists of a 10 nm GaAs capping layer, a 40 nm Si-doped AlGaAs, a 40 nm undoped AlGaAs and a thick GaAs substrate. The ionised dopants in AlGaAs build in electric fields and bend the conduction band. At the AlGaAs/GaAs heterointerface, the edge of the conduction band is pulled down to below the Fermi level, free electrons are introduced, and the wave functions are calculated by solving the 1D Schrödinger equation (seen inset B of Fig. 2.2(II). As shown in Fig. 2.2(II), due to the strong potential barrier in the growth direction at the interface, the free electrons are confined to a 2D plane, which is known as a 2DEG. A 40 nm undoped AlGaAs space-layer is designed to reduce the scattering from ionised Si dopants, and hence improve electron mobility in the 2DEG. Above, a thin GaAs layer is designed to prevent the oxidation of the Al atoms in the AlGaAs layer.

At a high temperature, above 100 K, by calculating electric fields at the surface (MBE regrown interface) and continuous charge displacement field, $D$, the surface charge density (back charge density) is calculated. Given a 2DEG density of $1.5 \times 10^{11}$ cm$^{-2}$, the surface charge density is around $-2.2 \times 10^{12}$ cm$^{-2}$ and the back charge state density is $5.5 \times 10^{10}$ cm$^{-2}$. Then, by delta-doping, the surface and back charges are implemented into the heterostructure. Finally, the simulation is repeated at a cryogenic temperature ($T = 4$ K) with the embedded surface and back charges frozen in.

Figure 2.2(III) depicts the band structure of an undoped GaAs/AlGaAs heterostructure. Unlike in the case of intentional modulation with Si atoms, a 2DEG is induced by external electric fields with surface metallic gates. As with the HEMT wafer, a 10 nm GaAs capping layer is designed to prevent the oxidation of Al atoms. A GaAs quantum well (QW) is sandwiched between two layers of AlGaAs of 90 nm
Chapter 2. Simulations of gate-patterned quantum devices

Figure 2.2: I: Schematic diagram of doped (A) and undoped (B) AlGaAs/GaAs heterostructures. The positions of 2DEG and the quantum well are indicated by the red lines. II: Conduction band as a function of depth Z. The surface charge (inset A) and back charge states are introduced at the surface and the MBE regrowth interface. Inset B: band edge at the AlGaAs/GaAs heterointerface with electron wave-functions at ground (yellow) and excited (blue) states. Inset C: 2DEG charge density as a function of depth. III: Band structures of the undoped AlGaAs/GaAs heterostructure. Inset A: when a positive voltage is applied to the surface gate, a 2DEG is induced in the QW. Inset B: when a negative voltage is applied by the surface gate, a 2DHG is induced in the QW.
and 300 nm-thick. The absence of intentional dopants gives a flat band and zero charge inside QW. When a positive bias of 0.8 V is applied to the metallic surface gate, the conduction band of the QW is bent below the Fermi level, inducing a 2DEG inside the QW (see inset A of Fig. 2.2(III)). Conversely, a negative voltage will raise up the valence band of the QW above the Fermi level, inducing a two-dimensional hole gas (2DHG) inside the QW (see inset B of Fig. 2.2(III)). In the QW, the electron and hole wave functions are calculated by solving the Schrödinger equation. To create a lateral $pn$ junction in a GaAs heterostructure, the QW needs to be narrow enough for the electron and hole wave-functions to overlap, which determines the probability of electron-hole recombination. Here we simulate the heterostructure with a QW of 15 nm.

This is straightforward for the one-dimensional structure simulation. However, when this is then transferred to three dimensions, the simulation is more complicated, particularly for the exposed surface between surface gates. The BCs we apply for 3D simulation become more important and also more difficult.

2.4 Simulation of 1D channel characterisation

![Diagram of split-gate device model](image)

Figure 2.3: Schematic diagram of the split-gate device model (a) with the electrostatic profile at the surface (b) and the 2DEG (c) for $V_{SG} = -1$ V.

We model a pair of split gates defining a narrow one-dimensional (1D) channel in the 2DEG of a Si-doped GaAs/AlGaAs heterostructure with a negative bias applied to the gates, $V_{SG}$, as shown in Fig. 2.3. Appendix A shows an example of a Nextnano input file for a split-gate device on a Si-doped AlGaAs/GaAs heterostructure. The heterostructure is the same as that in the 1D simulation. Instead of the direct BCs on the exposed surface, a vacuum or ‘air’ layer (a material with a large bandgap of 15 eV and a dielectric constant $\varepsilon = 1$) is introduced with Neumann BC $\partial \phi / \partial z = 0$ above the vacuum. As discussed above, the back BCs should be applied deep below
the regrowth interface. However, for these doped structures, we find no significant effect of moving the boundary from this interface. This is because, for there to be a charge in the 2DEG, there is a large built-in field above the interface even at high temperature, and this is screened by the charge at the regrowth interface, which then becomes frozen. Changing a surface gate voltage then causes a relatively minor shift in the bands, and taking the lower boundary any distance below the regrowth interface gives similar results.

The simulations are run with different values of $V_{SG}$ to check the electrostatic profile at the 2DEG, as shown in Fig. 2.4(a). As $V_{SG}$ becomes negative, the conduction-band minimum at the centre of the 1D channel begins to rise. When it is above the Fermi level, the electrons become fully depleted with the channel pinching off at $V_{SG} = V_P$, as shown in Figs. 2.4(b-e) for two different channel lengths $L$ (0.7 and 1.5 µm) but the same width $W$ (0.7 µm). The simulated $V_P$ is 1.16±0.02 V for a 1D channel of $L = 0.7$ µm and 0.89±0.02 V for $L = 1.5$ µm. This difference in $V_P$ come from the fringing field effect, the 1D channel we define has a finite length. The shorter the value of $L$, the more negative the $V_P$ that is required.

We find that there is no significant difference (within 2%) in both $V_P$ and the confining potential in the channel between a case in which the Neumann BC is applied on the exposed surface, and one in which there is a vacuum layer in between. This is because the large difference in the dielectric constant causes electric fields just inside the surface to be nearly parallel to it. As for the Neumann BC, if, instead, the vacuum region is replaced by a different dielectric layer with $\varepsilon \gg 1$, the result is different. The $V_P$ of the 1D channel of $L = 0.7$ µm varies from about $\sim -1.15$ V to $\sim -0.85$ V for $\varepsilon$ ranging from 1 (vacuum) to 13 (GaAs). Similarly the $V_P$ of a 1D channel of $L = 1.5$ µm varies from about $\sim -0.9$ V to $\sim -0.6$ V, as shown in the inset of Fig. 2.5 (b). For example, with a dielectric layer of ZnO ($\varepsilon = 8.3$), $V_P$ shifts by about 0.2 V, which should be observable in experiments.

### 2.4.1 Experiment to characterise 1D channels

For a comparison with the model, chips A and B were fabricated from a Si-doped GaAs/AlGaAs heterostructure containing a 2DEG situated 90 nm below the surface with density around $1.5 \times 10^{11}$ cm$^{-2}$ and mobility of $1.57 \times 10^{6}$ cm$^2$V$^{-1}$s$^{-1}$. Split gates were patterned using electron-beam lithography and metallised with Ti/Au (7/10 nm). A thick (1 µm) high-quality ZnO layer was deposited on chip B at room temperatures with a high-target-utilisation sputtering technique (HiTUS). To avoid unintentional accompanying ion implantation, which greatly reduces the 2DEG conductance, we deposit a thin (20 nm) amorphous aluminium oxide buffer layer using atomic-layer deposition after the gate metallisation but before the sputtering of ZnO. At $T = 4.2$ K, a source-drain current was driven by a 0.1 mV bias and the conductance, $G$, was measured with a lock-in amplifier at 77 Hz. Figures 2.5(a) and (b) demonstrate the pinch-off characteristics of different 1D channels in chips A and B with different dielectric layers above the surface. At $V_{SG} = -0.2$ V, the 2DEG under the gate is depleted, defining the 1D channel, and the channel is finally pinched off at $V_{SG} = V_P$. At $-0.89 \pm 0.05$ V (−1.15 ± 0.05 V), the 1D channel created by split gates $L = 1.5$ µm ($l = 0.7$ µm) is pinched off. The error bar in $V_P$ is derived from an average of multiple sweeps. $V_P$ is dependent on the length of the
Figure 2.4: (a) 2D electrostatic map of the 2DEG with $V_{SG} = -1.1\,\text{V}$ in a split gate device with $L = 0.7\,\mu\text{m}$. (b) and (c): 1D electrostatic energy profile along and across a 1D channel of $L = 0.7\,\mu\text{m}$, following the white and red lines in (a), at $V_{SG}$ from 0 to $-1.3\,\text{V}$. (d) and (e): 1D electrostatic energy profile along and across the 1D channel of $L = 1.5\,\mu\text{m}$ at $V_{SG}$ from 0 to $-1.1\,\text{V}$. 

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Table 2.1: Comparison of experimental and simulated pinch-off voltages.

<table>
<thead>
<tr>
<th>Dielectric</th>
<th>$L$ ($\mu$m)</th>
<th>$V_P$: experiment (V)</th>
<th>$V_P$: simulated (V)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Air</td>
<td>0.7</td>
<td>$-1.15 \pm 0.05$</td>
<td>$-1.16$</td>
</tr>
<tr>
<td>Air</td>
<td>1.5</td>
<td>$-0.89 \pm 0.05$</td>
<td>$-0.9$</td>
</tr>
<tr>
<td>ZnO</td>
<td>0.7</td>
<td>$-0.88 \pm 0.03$</td>
<td>$-0.92$</td>
</tr>
<tr>
<td>ZnO</td>
<td>1.5</td>
<td>$-0.60 \pm 0.03$</td>
<td>$-0.68$</td>
</tr>
</tbody>
</table>

1D channel, becoming more negative for a shorter lithographic channel length $L$, which matches the simulation results.

In chip B, the ZnO overlayer leads to a $\sim 0.25$ V shift of $V_P$ towards zero, compared with chip A. The quasi-1D channel created by split gates $L = 1.5 \mu$m ($L = 0.7 \mu$m) is fully pinched off at $-0.6 \pm 0.03$ V ($-0.88 \pm 0.03$ V). To exclude the possibility of ‘damage’ occurred to the 2DEG during deposition, we etched the ZnO layer on chip B with 20% HCl solution (chip B’ in Fig. 2.5(b)). $V_P$ became comparable to the values for chip A (the remaining slight difference can be explained by the presence of the thin Al$_2$O$_3$ buffer layer). As shown in Table 2.1, the experimental results for $V_P$ match the calculation very well, in particular having the same shift when there is a ZnO layer. This shows that it is essential to take into account the effect of the dielectric layer.

There are limitations in comparing theory and experiment. Experimentally, for a 1D channel, $V_P$ is affected by wafer disorder, lithographic imperfections, device cool-down rate, sweep direction and sweep rate. There are also uncertainties in the dielectric constant and Schottky barrier energy for ZnO grown by HiTUS, as they are dependent on surface conditions, crystal quality, etc. In MBE growth, there is a low but uncertain density of unintentional dopants in heterostructures, typically $p$-type from carbon atoms. In Table 2.1 we compare $V_P$ with and without $10^{13}$ cm$^{-3}$ fully-ionized $p$-type dopants, and the errors indicate the spread between these two cases. However, the error in $V_P$ caused by this uncertainty is much smaller than the measured errors with and without the ZnO overlayer, proving the importance of the boundary condition at the surface.

### 2.5 Simulation of an induced lateral $n$-$i$-$n$ junction

For a more sensitive test of BCs, we consider the second type of gated device on an undoped GaAs/AlGaAs heterostructure. Figure 2.2(III) illustrates the conduction band of such a heterostructure. An external electric field applied by a surface inducing gate pulls the conduction (valence) band below (above) the Fermi level, inducing free electrons (holes) inside a quantum well (QW). The carrier density of this 2D gas is tuned by gate bias instead of doping density. This inducing technique greatly reduces the density of ionised scatterers and gives high carrier mobility with a low carrier density. With a positive bias on the two inducing gates ($V_I > 0.8$ V) separated by 600 nm, electrons accumulate under each inducing gate, forming a source and drain separated by an intrinsic barrier (a lateral $n$-$i$-$n$ junction). The electrostatic potential distribution through the $n$-$i$-$n$ junction is calculated using our model (as shown in Fig. 2.6(a)) and verified experimentally by using a surface
Section 2.5. Simulation of an induced lateral \textit{n-i-n} junction

Figure 2.5: (a) Pinch-off characteristics of chip A with an air dielectric layer. Inset: the conduction band minimum of the centre of a 1D constriction of dimensions $L = 0.7 \mu m$ (red triangles) or $L = 1.5 \mu m$ (black circles) as a function of $V_{SG}$. (b) Pinch-off characteristics of chip B with a ZnO dielectric layer (thick line) and chip B’, the same chip after etching off the ZnO again (thin line). Inset: calculated pinch-off voltage of a 1D channel with $L = 1.5 \mu m$ (black circles) or $L = 0.7 \mu m$ (red triangles) as a function of the dielectric constant of a dielectric layer (of thickness 1 \mu m).
acoustic wave (SAW) to pump electrons across the potential hill in the intrinsic region.

If the maximum slope in the potential hill is lower than that in the SAW, the SAW can collect electrons and drag them up and down the hill.\textsuperscript{79,80} Assuming that a SAW potential is a sine wave, the required SAW amplitude is estimated from the electrostatic energy profile through the $n$-$i$-$n$ junction. Unlike in the case of a doped device, there are no built-in electric fields in an undoped device, and so there are no frozen charge layers on either the front or back surfaces. This means that the choice of BCs is more important in an undoped device than in a doped one. Here we have ignored the unintentional impurities from the MBE chamber because of uncertainties in terms of the density and complicated dopants. A similar result is found when comparing the model with and without unintentional $p$-type dopants at a density of $10^{13}$ cm$^{-3}$.

To induce a 2D gas, we apply an inducing-gate voltage, causing a large electric field below the surface, as well as above the surface. Thus, one should include a dielectric layer and set a Neumann BC at the top of the dielectric layer, as described above. In a model of a doped device, we find that the position of the back BC is not important. However, the lack of back-charge states in an undoped device can help in probing the back BC. If one assumes that the bands are pinned at the regrowth interface a few microns below the surface, the maximum potential slope in the $n$-$i$-$n$ junction is so large that a SAW with an amplitude greater than 100 meV appears to be required to pump electrons.
Section 2.5. Simulation of an induced lateral $n$-$i$-$n$ junction

On a GaAs substrate for similar SAW devices, the SAW amplitude was measured at around 20–30 meV at a power of 8–10 dBm.\textsuperscript{80–82} Given this, it should be impossible to realise SAW pumping in a such an induced $n$-$i$-$n$ junction, which conflicts with our experimental observations. Figure 2.7(a) illustrates the calculated potential through the $n$-$i$-$n$ junction for various depths, $d_{sub}$, of the back BC. As $d_{sub}$ increases, the required SAW amplitude decreases significantly and stabilises at around 25 meV for depths over 20 $\mu$m (inset to Fig. 2.7(a)). This saturation depth is strongly dependent on the dimensions of the intrinsic region. A larger $d_{sub}$ is required for a wider intrinsic gap in a $n$-$i$-$n$ junction.

Figure 2.7: (a) Conduction band energy profile through a lateral $n$-$i$-$n$ junction with different depths from the back surface $d_{sub} = 2, 3, 5, 7, 10, 20, 30$ and 50 $\mu$m at $V_i = 1.2$ V and $V_{SG} = 0$. The Fermi level is taken to be 0. Inset: required SAW amplitude $A_{SAW}$ as a function of $d_{sub}$. (c) Required SAW amplitude ($d_{sub} = 50$ nm) as a function of $V_{SG}$ at different $V_i$ of 1 V (blue triangles), 1.1 V (black squares), and 1.2 V (red circles).

To manipulate the SAW pumping process in the simulation, we place a pair of split gates on the sides of the intrinsic region (inset of Fig. 2.7(b)). We simulate the approximate required SAW amplitude as a function of $V_{SG}$ and $V_i$, as shown in Fig. 2.7(c). As $V_{SG}$ becomes more negative, the channel is squeezed, and the potential hill becomes higher, making SAW pumping harder, as shown in Fig. 2.6(b). When increasing $V_i$, the induced 2DEG density and Fermi energy increase and the source and drain regions expand, pulling down the potential hill so that the slope
above the Fermi level is less, making SAW pumping easier. For $V_I = 1.2 \text{ V}$ and a SAW amplitude of $40 \text{ meV}$, the threshold (pinch-off) split-gate voltage for SAW pumping is $V_P = -0.27 \text{ V}$. Close to the pinch-off, the transverse confinement is strong enough to define a dynamic quantum dot (DQD) in each SAW minimum, containing a precise number, $n$, of electrons, as the Coulomb charging energy is sufficient to prevent confinement of an extra electron. This has been shown to give a quantised acoustoelectric current $I = n e f$, where $f$ is the SAW resonant frequency.\textsuperscript{21,83}

### 2.5.1 Experimental investigation with SAWs

Dr. Yousun Chung fabricated an induced lateral $n$-$i$-$n$ junction device on an undoped GaAs/AlGaAs heterostructure with a quantum well width of 15 nm located 100 nm below the surface, which is the same as that in the 1D simulation.\textsuperscript{84} In the device, AuBe, as $p$-type Ohmic contact metal, was evaporated and annealed at $520 \degree \text{C}$ for 90 s. AuGeNi, as $n$-type Ohmic contact metal, was evaporated and annealed at $460 \degree \text{C}$ for 80 s. There are three types of metallic surface gates: bridging gates, inducing gates, and split gates. The bridging gate applies a strong electric field through a thick insulator (Polyimide HD4014) to induce electrons or holes around the Ohmic contacts. The inducing gate is used to drag the electrons or holes outside the Ohmic contacts and accumulating under the gates, which creates an induced lateral $n$-$i$-$n$ or $n$-$i$-$p$ junction. Another pair of split gates at the centre of the chip is used to control the junction separately and provide transverse confinement. A SAW resonant at $f = 2.8 \text{ GHz}$ is launched by an IDT with period of $1 \mu \text{m}$.

Figure 2.8(a) illustrates the induced device in an undoped GaAs/AlGaAs heterostructure with a lateral $n$-$i$-$n$ junction, matching the modelled device. At a low temperature of $T = 4.2 \text{ K}$ and an inducing-gate voltage $V_I = 1.2 \text{ V}$, a strong SAW overcomes the potential hill in the intrinsic region and drags electrons from source to drain, exhibiting quantised acoustoelectric current as a function of $V_{SG}$ at different SAW powers from 10.5–12 dBm, as shown in Fig. 2.8(b). This measurement was done by Dr. Yousun Chung. The dashed lines in Fig. 2.8(b) show the expected positions of the first two plateaux at $I = e f \sim 0.45 \text{ nA}$ and $I = 2e f \sim 0.90 \text{ nA}$. The threshold pinch-off voltage $V_P$ ranges from $-0.12 \text{ V}$ at a SAW power of $11 \text{ dBm}$ to $-0.33 \text{ V}$ at $12 \text{ dBm}$, which corresponds to a change in amplitude of a factor of 1.12. The model in Fig. 2.7(c) shows the same trend in $V_P$, but such a change in $V_P$ requires a larger increase in SAW amplitude than in the experiments. This can probably be explained by a charging effect that caused a drift of $V_P$ in this sample.

We notice that the first plateau is visible at $V_{SG} = 0 \text{ V}$ (at a power of $11 \text{ dBm}$), which shows that there is strong transverse confinement even with a grounded split gate; the split gates screen the field from the inducing gates, so that, close to the side gates, the bands are not as close to the Fermi energy. Our calculation at $V_{SG} = 0 \text{ V}$ also gives transverse confinement, which fits a parabolic potential with a single-particle energy-level of $1 \text{ meV}$. This shows that grounded gates and exposed surfaces behave differently in undoped material, whereas in doped heterostructures there is usually very little difference.
Section 2.5. Simulation of an induced lateral $n$-$i$-$n$ junction

![Scanning electron micrograph of an induced SAW device](image)

**Figure 2.8:** (a) Scanning electron micrograph of an induced SAW device. (b) Quantised SAW-driven current $I_{SAW}$ in a lateral $n$-$i$-$n$ junction ($V_I = 1.2$ V) as a function of $V_{SG}$ for different RF powers. Inset: SEM image of the junction. (c) Calculations matching the experimental device for $d_{sub} = 50 \mu m$ and $3 \mu m$: a SAW (amplitude 25 meV) is superimposed on the potential ($V_I = 1.2$ V, $V_{SG} = 0$ V). Minima form on either side of the intrinsic barrier, and the curves show the numbers $N_L$ and $N_R$ of electrons in them as a function of time as the SAW moves to the right. Arrows after each step show the direction in which that electron tunnels out of the left dot. Inset: 2D combined potential (top) and 1D profiles along the junction with (blue) and without (black) the SAW.
2.5.2 Quantised charge transport

In order to explain the quantised acoustoelectric current, we use a simple model in which electrons in a SAW-driven dot can tunnel out via saddle-point potential barriers. The transmission probability through such a barrier with potential \( V(x, y) = V_0 - \frac{1}{2}m^*\omega^2_x + \frac{1}{2}m^*\omega^2_y \) is

\[
T = \frac{1}{1 + e^{-\pi\epsilon}}
\]

where

\[
\epsilon = \frac{2(E_N - \frac{1}{2}\hbar\omega_y - V_0)}{\hbar\omega_x},
\]

and \( m^* \) is electron effective mass.\(^{85,86}\) We superpose a SAW potential on to the calculated electrostatic potential and calculate \( \omega_x \) for the barriers, together with the energy of the \( N^{th} \) electron, \( E_N \), which is estimated from the electron ground-state energy in the SAW minimum and a constant Coulomb charging energy, taken to be 3\,meV.\(^{29}\) However, the actual process of SAW pumping is much more complicated. The size of the dot changes throughout the process of climbing the intrinsic barrier. Hence the charge energy is not a constant. Moreover, the rapid change in the potential of the quantum dot causes adiabatic errors, as the electron is excited from the ground state to the excited states. To simplify the model, all these effects are excluded.

In studies of quantised SAW pumping in doped devices, the barrier is usually longer than the SAW wavelength. Therefore, only back-tunnelling is generally considered.\(^{21}\) However, for the short intrinsic channel used in this experiment, we need to calculate tunnelling processes through both the back and front barriers. Our model shows that it is still possible, and likely, that electrons in the SAW minimum, which we label L, will tunnel forwards into the minimum ahead of the intrinsic barrier, which we mark R, provided we use deep BCs. Firstly, for a deep BC, \( d_{sub} = 50\,\mu m \) (solid lines). During a SAW cycle, \( N_L \) decreases as electrons tunnel back to the source through the back barrier. However, at some point (\( t = 7\,ps \) in the plot) the probability of forward tunnelling through the front barrier becomes greater than that of back-tunnelling, causing confinement to decrease and the electrons trapped in the dot to tunnel forwards, increasing \( N_R \) (upper inset). Later, at around 15\,ps here, the right dot begins to rise again so that forward tunnelling stops, and back-tunnelling starts again. Eventually, the left dot empties. This results in an integer number of electrons being pumped through the intrinsic region in each SAW cycle, yielding a quantised current.

In contrast, for shallow BCs (\( d_{sub} = 3\,\mu m \), shown with dashed lines), the front barrier is so high that electrons in a SAW minimum tunnel back to the source through the back barrier (lower inset). Therefore \( N_R = 0 \) over a whole SAW cycle, which is not reflected in the experiment. In reality, metal gates and free charges screen and attenuate the SAW,\(^{86}\) whereas we assume a constant SAW amplitude in the above model. The screening will only reduce the chance of pumping for a given applied SAW amplitude, so with shallow back BCs it would still be impossible to pump electrons. Deep BCs are vital to explaining our experimental observations of pumping, and this highlights the important role of freezing of charge at the regrowth.
interface in patterned devices on undoped (and doped) heterostructures, which has mostly been ignored in the past.

2.6 Simulation of an induced lateral $n$-$i$-$p$ junction

One of the advantages of induced devices is flexibility. When we reverse the sign of the inducing-gate voltage to negative, electric fields pull up the valence band. When $V_I$ reaches around $-0.8\, \text{V}$, the valence band rises and the edge of the valence band of the quantum well come above $E_F$, inducing a 2DHG. By simply varying the inducing-gate voltage, the lateral induced $n$-$i$-$n$ junction is converted to an induced lateral $n$-$i$-$p$ junction. When a large forward bias (greater than the GaAs bandgap) is applied, electrons in the source diffuse to the drain and recombine with holes. This electron-hole recombination generates photons with energy matching the band gap of the GaAs QW. As shown above, SAWs cause the quantised pumping in an induced lateral $n$-$i$-$n$ junction. In this case, we can control the process of electron-hole recombination with SAWs by confining an integer number of electrons in each SAW minimum. When there is only one electron in each SAW minimum, a single-photon source with a high repetition rate of SAW frequency may be achieved. Figure 2.9(a) shows the electrostatic energy profile of the lateral $n$-$i$-$p$ junction with superposition of SAWs with a wavelength of $1\, \mu\text{m}$ and an amplitude of $40\, \text{meV}$.

![Figure 2.9(a)](image)

Figure 2.9(a): Schematic diagram of SAW-driven single-photon source through a lateral induced $n$-$i$-$p$ junction, electrons (red balls) are collected in SAW minima, As they pass the intrinsic barrier, the SAW minima are modulated, and electrons with high energy are forced out (yellow balls). Only one electron finally recombines with holes (blue balls).

In a simulation of an induced lateral $n$-$i$-$n$ junction, we only solve the electrostatic Poisson equation. However, in a simulation of an induced lateral $n$-$i$-$p$ junction, we need to solve the coupled Current-Poisson equations with Nextnano, which separates the electron and hole Fermi levels. In the calculation, double self-consistent processes are performed: one is for the electrostatic potential and density, and the other is for the Fermi levels of holes and electrons.

We first performed an induced lateral $n$-$i$-$p$ simulation with improved boundary conditions, in particular, a deep boundary condition on the back surface. When a positive voltage is applied to the electron inducing gate $V_I = 1\, \text{V}$, electrons are induced and accumulate under the gates, which works as a source (see inset of Fig. 2.9(b)). Similarly, when a negative voltage is applied to the hole inducing gate, $V_I = -1\, \text{V}$, holes are induced and accumulate underneath the hole inducing gate.
Figure 2.9: (a) Electrostatic profile of an induced lateral $n$-$i$-$p$ junction with the superposition of a SAW with its 1D cut along (red dashed line) and across (white dashed line) the junction. (b) Band structure of an induced lateral $n$-$i$-$p$ junction with the symmetric bias of 1.4 V. Inset: the edge of the conduction band below the Fermi level. Electrons are accumulated. (c) Electrostatic profile along an induced lateral $n$-$i$-$p$ junction at different value of $V_{SG}$ from 1 V to $-1$ V. Inset: the required SAW amplitude for pumping the intrinsic barrier as a function of $V_{SG}$. 
which works as a drain. Due to the large effective mass of holes, their Fermi energy is only one-fifth of the electron Fermi energy for the same carrier density.

There are two ways to apply a forward source-drain bias: symmetric and asymmetric. For a total forward bias of 1.4 V, we apply a 1.4 V bias directly to the drain (asymmetric), or alternatively we apply −0.7 V to the source and then 0.7 V to the drain (symmetric). In the doped n-p junction, these two methods will work in the same way. In an induced n-i-p junction, the electron and hole densities are controlled by the inducing gate voltage. When we use a symmetric bias, the inducing gate voltage is still referred to the zero Fermi level. However, if we use an asymmetric bias, the inducing-gate voltage needs to be adjusted according to the different references. In the asymmetric bias, carriers may eject into the intrinsic region from the split gates. Therefore the symmetric bias is preferred in both experiments and simulations. Figure 2.9(b) shows the band structure of an induced lateral n-i-p junction with a symmetric bias of 1.4 V. With a SAW of amplitude 40 meV, it is possible for electrons to be dragged across the intrinsic barrier by a SAW and then to recombine with holes. This SAW-driven photon source has been experimentally observed in our group. As similar with an induced n-i-n junction, if a shallow back boundary condition is chosen, the intrinsic barrier becomes much higher, and it is impossible for a SAW with the same amplitude to pump electrons across the intrinsic barrier. These measurements and simulations again prove the importance of back boundary conditions in an undoped device.

To achieve a single-photon source, a pair of split gates is needed beside the intrinsic region, which is similar to the n-i-n junction. Figure 2.9(c) shows the electrostatic energy profile along an induced lateral n-i-p junction at different $V_{SG}$. From the maximum gradient of the profile, we can calculate the required SAW amplitude in different conditions, with both positive and negative $V_{SG}$ modulating the intrinsic barrier, and hence the SAW longitudinal confinement. However, making $V_{SG}$ negative provides transverse confinement of electrons, which is important for quantised charge pumping. By applying a negative $V_{SG}$, the number of electrons in a SAW minimum can be manipulated, perhaps to reach the single electron regime. Figure 2.10 shows the schematic process in the evolution of dynamic quantum dots, leaving only one electron in the SAW minimum for a single-photon source. However, in an induced lateral n-i-p junction, the strong negative voltage on the split gates also induces holes under the gate when $V_{SG} < 0.8$ V, which may cause a serious leakage problem in experiments. To prevent this, we define an etched region outside the junction, which is etched down through the QW, as in the experimental device.

In an undoped n-i-n device, because of the screening of the electric field, grounding split gates also provide transverse confinement. As with an undoped n-i-p junction, the influence of the split gate become more obvious than the undoped n-i-n junction. The split gates are in an etched region and close to the QW, and hence the screening of electric fields becomes stronger. The inset of Fig. 2.9(c) shows the required SAW amplitude as a function of $V_{SG}$, as well as the minimum at $V_{SG} = 0$ for a device without etching. Because of the stronger screening effect in the etched devices, the minimum is shifted to $V_{SG} \sim -0.5$ V, which is also observed in experimental measurements by Dr. Tzukan Hsiao.44

In experiments with the induced n-i-p junction, the SAW-driven quantised electron transport has not been observed. From the simulation, we find that the trans-
verse confinement comes mainly from the etched channel, rather than from split gates. Due to the channel being around 1.2 µm wide, the transverse confinement, $\hbar \omega_y$, of only 0.1-0.2 meV, is not strong enough to define a dynamic quantum dot. This simulation result explains why the SAW-driven quantised current is not observed in experiments. To provide stronger transverse confinement, a narrow etched channel with a width of 200 nm can be used in the simulation. However, in experiments, this is not easy to achieve. A chemical etching process with such a narrower channel is difficult to control. However, it does not influence the observation of photon anti-bunching. When the SAW-pumping current is controlled at or below $1 e_f$, the photon anti-bunching with $g^{(2)} = 0.39$ was observed. To improve the quality of the SAW-driven single-photon source with a lower $g^{(2)}$, a further attempt at the transverse confinement enhancement is still important, by using the simulations to design better device.

### 2.7 Summary

To conclude, we have compared experiments on gate-patterned quantum devices at cryogenic temperatures with self-consistent electrostatic modelling using various boundary conditions and standard software. The models are fairly accurate, provided the boundary conditions are chosen carefully. For real 1D channels in a doped GaAs heterostructure, the pinch-off voltage shifts by $\sim 0.2$ V after depositing a ZnO layer. In order to account for this in our model, we have to treat the surface of the GaAs as having a frozen surface charge layer, rather than simply making it satisfy particular boundary conditions below the dielectric layer. To refine the back BCs, we compared modelling and experiments involving pumping electrons through an induced quantum device in an undoped GaAs heterostructure. In a lateral $n-i-n$ junctions, the SAW quantised charge transport is observed. To model the quantisation, we find that it is important to move the back boundary much deeper than the MBE regrowth interface, which has often been taken as an equipotential. In the simulation of a lateral $n-i-p$ junctions, we verify the possibility of pumping electron across the junction, and also explain why the quantised pumping current can not be observed in the experiment with the weak transverse confinement. With these improved boundary conditions, it is possible to produce an accurate model and to optimise complex gate-patterned quantum devices. These numerical simulations show great potential in terms of the device design and optimisation, and pave the way for a high-quality SAW-driven single-photon source.
3.1 Motivation

In the quantum metrological triangle of Ohm’s law, the SI unit of resistance, the ohm (Ω), is defined by the Hall resistance, $R_H = \frac{h}{e^2}$, from quantum Hall measurements with a relative uncertainty of two parts in $10^8$. The SI unit of voltage, the volt (V), is defined by the Josephson constant, $K_J = \frac{2e}{h}$, from the Josephson effect with a relative uncertainty of five parts in $10^7$, where $e$ is the elementary charge and $h$ is Planck’s constant. The SI unit of current, the ampere (A) is defined by the force between two parallel conductors in a finite length. In this triangle, the definition of ampere is not as flexible as the ohm and the volt using the Hall resistance and Josephson constant. Then the single-electron transport is proposed to redefine the ampere using $I = \frac{ef}{N}$, where $f$ the frequency and $e$ is the elementary charge. Now the single-electron transport can reach a relative uncertainty of 2 parts in $10^7$.

Surface acoustic waves (SAWs) have shown strong abilities in single electron manipulation. In an AlGaAs/GaAs heterostructure, SAWs have achieved quantised electron pumping. This SAW quantised pumping could be used in the quantum metrological triangle. However, the best precision on SAW plateaus is about 60 parts in $10^6$ and is not good enough to redefine the ampere.

In a gate-defined charge pump, instead of using SAWs, an AC voltage is directly applied to a gate to generate dynamic quantum dots (DQDs) and quantised pumping current $I = Nef$, as shown in Figs. 3.1(a-c). In this charge-pumping experiment, the accuracy of quantisation was found to be highly improved by the application of a strong out-of-plane magnetic field. In a strong magnetic field up to 14 T, the accuracy of quantisation improved to parts in million, which is close to the accuracy requirement for metrological applications, as shown in Fig. 3.1(d). Theoretically, in a saddle-point potential model and a one-dimensional WKB approximation, the electron tunnelling rate is given by:

$$T(E) \simeq e^{-2f \int \sqrt{\frac{2m^*}{\hbar^2}(V(x)-E)}dx}$$

where $m^*$ is effective electron mass, $V(x)$ is the potential barrier, and $E$ is the electron energy. In DQDs, we assume there is a simple harmonic oscillator with ground-state energy $(1/2)\hbar\omega_0$ and energy spacing $\hbar\omega_0$. The charge quantisation in dynamic quantum dots comes from the different tunnelling rates of the $(N+$
Chapter 3. Energy spectroscopy of SAW-driven quantum dots

Figure 3.1: Scanning electron microscope image of the gate-defined charge pump (a) and schematic electrical connections (b). Electrons are pumped from left to right. (c) Potential profile during the pumping cycle (offset vertically): (i) loading, (ii) back-tunnelling, (iii) trapping, and (iv) forward-tunnelling. (d) First quantised plateau at different magnetic fields from 0 to 14 T. (e-f) Differential current as a function of gate voltage and magnetic fields at different operating frequencies: 0.1 GHz, 0.4 GHz and 1 GHz. Figures from Ref. 90.
1)th electron and the Nth electron in the dots. When the (N + 1)th electron in a dot tunnels out and the Nth electrons is still inside the dot with lower tunnelling probability, the ratio of the tunnelling rate of the (N + 1)th electron and the Nth electron \( \Gamma_{N+1}/\Gamma_N \) will control the accuracy of the charge pumping quantisation. Under a strong magnetic field, both \( \Gamma_N \) and \( \Gamma_{N+1} \) decrease, but \( \Gamma_{N+1}/\Gamma_N \) increases and better quantisation should be observed in the Nth plateau than it without magnetic fields. For a constant barrier potential \( V_0 \) of width \( d \), Eqn. 3.1 is simplified to:

\[
\Gamma \propto e^{-\frac{2\sqrt{2m^*}}{\hbar^2} \left( V_0 - E \right)}.
\]

(3.2)

In this expression, the log of the ratio of the tunnelling rates is given by:

\[
\delta = \ln \Gamma_{N+1} - \ln \Gamma_N = \frac{d}{\hbar \sqrt{2m^*}} \frac{\sqrt{V_0 - E}}{\Delta},
\]

(3.3)

where \( \Delta \) is the quantum-dot charging energy. In magnetic fields, the electron wave function shrinks, which is equivalent to widening the tunnelling barrier. Here an effective width \( d_e \) is defined as a function of magnetic field.\(^{95,96}\)

\[
d_e = d - \ell_B(B) + \ell_B(0)
\]

(3.4)

\[
\ell_B(B) = (m^* (\sqrt{\omega_0^2 + \omega_c^2/4}/\hbar))^{-1/2}
\]

(3.5)

where \( \omega_c = eB/m^* \). As \( B \) increases, \( \delta_B/\delta_0 \sim d_e(B)/d_e(0) \) will increase, which will result in a better quantisation, in theory. Both experiments and theories show that a strong perpendicular magnetic field will suppress the tunnelling rate, and give better quantisation. By measuring the single-electron wave packets in the charge pump, Fletcher et al. found that the electron difference for the first electron and second electron in the dynamic quantum dot can be around 8 meV.\(^{97}\) For the charging effect, a larger addition energy in the quantum dot will contribute to a better quantisation.

In a standard gate-defined charge pump, the accuracy of quantisation is also dependent on the operation frequency. A charge pump at 0.1 GHz shows better quantisation than it does at 1 GHz, as shown in Figs. 3.1(e-g).\(^{90}\) At low frequencies, we can take the pumping process as an adiabatic process (the change of potential is slow enough). However, at 1 GHz, the quantised current \( I = Ne f \) is supplemented by a non-adiabatic contribution.\(^{98}\) Kataoka et al. observed tunable non-adiabatic excitation in high-frequency charge pumping in magnetic fields, as shown by ‘L1’ in Fig. 3.1(g).\(^{99}\) They showed that the non-adiabatic excitation severely damages the quantisation accuracy of a high-frequency pump. In our SAW-pumping experiments, we apply a 3 GHz SAW and a non-adiabatic effect should be considered. Flensberg et al. calculated the non-adiabatic effect in electron transport driven by SAWs.\(^{100}\)

When the gate voltage, \( V \), is close to the Nth plateaus, the slope of the plateau is expressed by:

\[
S = \frac{1}{I_0} \left( \frac{dI}{dV} \right)_{V \rightarrow N} \approx (2Ec/k_B T_{\text{eff}}) e^{-Ec/k_BT_{\text{eff}}}
\]

(3.6)

with

\[
T_{\text{eff}} = \sqrt{T^2 + (0.88\hbar/k_B\tau)^2}.
\]

(3.7)
Here $I_0$ corresponds to the perfect quantisation, $E_C$ is the charging energy and $\tau$ is the characteristic time defined by:

$$\tau \approx \frac{l_0}{v_s},$$

(3.8)

where $l_0$ is the distance the electron wave function leaks outside the barrier, and $v_s$ is the SAW velocity (2800 m/s for GaAs). As $B$ increases, the electron wave function shrinks and $l_0$ becomes short, and as $\tau$ then decreases, the slope of the plateau drops.

According to these, we design an energy spectroscopic experiment to probe electron energy in a SAW-driven dynamic quantum dot and try to understand error mechanisms of SAW quantised pumping. We also discuss the magnetic-field dependence of SAW quantised current in both experiment and theory.

### 3.2 Device fabrication and characterisation

SAW devices are based on a GaAs high-electron-mobility-transistor (HEMT), including mesa, Ohmic contacts, gates, and inter-digital transducers (IDTs). High-quality HEMT wafers are grown using molecular beam epitaxy (MBE). In this work, we use wafers W552 and W886 (data sheet in Table 3.1). The electron density ($n_{2D} \simeq 1.6 \times 10^{11}$ cm$^{-2}$) and mobility ($\mu \simeq 1.6 \times 10^6$ cm$^2$ V$^{-1}$ s$^{-1}$) are almost the same in the two wafers, so the result should be comparable. SAW propagation requires a good smooth surface, any residues or scratches will attenuate the SAW. Hence much care is needed during fabrication.

<table>
<thead>
<tr>
<th>Wafer</th>
<th>Carrier density (cm$^{-2}$)</th>
<th>Mobility (cm$^2$ V$^{-1}$ s$^{-1}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>W552</td>
<td>$1.71 \times 10^{11}$</td>
<td>$1.59 \times 10^6$</td>
</tr>
<tr>
<td>W886</td>
<td>$1.59 \times 10^{11}$</td>
<td>$1.57 \times 10^6$</td>
</tr>
</tbody>
</table>

measured at 1.5 K in the dark

#### 3.2.1 Mesa etching

Once a high-quality wafer is selected, a large piece of material is cleaved from the wafer using a diamond-tipped scribe and cleaned with acetone and isopropyl alcohol (IPA) for a few minutes in an ultrasonic bath. Then we pattern a mesa using optical lithography and chemical etching, as seen in Fig. 3.2. Firstly, the chip is put on a hot plate ($115^\circ$C) for 2 mins to remove any residual solvent. It is then moved to a spinner. A few drops of Shipley-1813 photoresist are deposit to cover the whole chip, and the chip is spun at 5500 rpm for 30 s, creating a uniform thin layer (around $1 \mu$m) of photoresist on the chip. After the back of the chip has been cleaned with acetone, it is re-baked at 115°C for another 1 min. If any acetone accidentally contaminates the surface photoresist, we have to clean the chip with acetone and IPA and repeat the above processes.

A chrome-on-quartz mask provides mesa patterns. After cleaning with acetone and IPA, we mount the mask on an aligner with the chrome-coating side down.
The chip is put on a stage and aligned with the mesa pattern. The SAW propagation direction is highly dependent on a particular crystal axis, and hence the alignment of SAW devices is essential: the high mobility direction is aligned with the SAW propagating direction. Furthermore, a 1 mm gap is left to avoid edge-bead effect (non-uniformity of the spinning photoresist at the edge of the chip) and also to make it easy for holding with Teflon-coated tweezers. After precise alignment, the stage is raised to bring the chip into contact with the mask. It is then exposed to UV light for 6.5 s. After being developed with MF319 photoresist developer for 30 s, as well as rinsing with deionised (DI) water and drying with N₂, we check the pattern under a microscope. The photoresist is strongly sensitive to UV-light, and hence the optical lithography must be performed in a yellow room, for which UV light is excluded. Only after it is fully developed can a chip with photoresist be taken outside the yellow room.

A Dek-Tak surface profiler is used to scan a few selected paths and gives a reference height for chemical etching. Before etching, we remove surface oxide by dipping the chip into 10% HCl for 20 s. We use an etching solution of H₂SO₄ : H₂O₂ : H₂O = 1 : 8 : 111. The etch rate is sensitive to the etchant temperature, and may also differ from wafer to wafer. It is necessary to dip the chip for 5 s to determine the etch rate with the Dek-Tak profiler, which is usually around 10 nm/s. Then according to this rate, we re-dip the chip into the etching solution. To ensure the 2DEG is fully removed outside the mesa, we etch over 100 nm deep, making sure the entire AlGaAs layer is etched away. Finally, the photoresist is stripped with acetone. The actual etch depth is measured with the Dek-Tak profiler again. Sometimes, the etching depth measured with and without the photoresist is different, which may come from non-uniformity of the photoresist layer. Adequate etching is important to remove the 2DEG in the SAW propagation path. If the etching is not sufficient, the continuous 2DEG and the oxidisation of the AlGaAs layer attenuate SAW propagation.

### 3.2.2 Ohmic contacts

Ohmic contacts are electrical contacts, obeying Ohm’s Law, used to measure electron transport in a 2DEG. As with the mesa, we pattern Ohmic contacts using optical lithography (Figure 3.3 (b)), followed by spinning, alignment, exposure and development. Before mounting into a thermal evaporator, we use oxygen plasma ashing for 1 min and 10% HCl solvent for 20 s to remove the photoresist residue and
oxide on the surface. AuGeNi alloy (around 500 mg) is put into an evaporator. After pumping down to a low pressure of $2 \times 10^{-6}$ mbar, 100-150 nm metal is deposited at a rate of 0.5 nm/s, which is controlled by the applied current. It is important to evaporate all of the alloy, as any residue of the alloy will contaminate the subsequent evaporation. After evaporation, the chip is soaked in acetone for lift-off process (a few seconds of ultrasonic bathing is helpful), leaving the Ohmic contacts on the chip. We check the lift-off quality under a microscope with the chip just covered by IPA, so the lens is not immersed by IPA. Once good lift-off is confirmed, the chip is moved from IPA and dried with N$_2$.

After the lift-off, the chip is annealed at 430°C for 80 s in a rapid thermal annealer. At high temperatures, germanium atoms diffuse down to the GaAs layer and dope GaAs an $n$-type semiconductor, creating Ohmic contacts. After annealing, the colour of the Ohmic contacts is slightly different under a microscope. The quality of Ohmic contacts is checked using microscopic probe tips, which connect with a multimeter. The resistance between the two Ohmic contacts in a device is $\sim 20 \, k\Omega$ at room temperature. If the chip is cooled down to 77 K by pouring liquid nitrogen over it, the resistance decreases to $\sim 2 \, k\Omega$. In this process, the light from the microscope should be turned off to exclude any photovoltaic effect.

### 3.2.3 Surface gates

Surface metallic gates are used to apply external electric fields to the 2DEG but are not directly in contact with the 2DEG. Since the UV photon wavelength is around 0.3 $\mu$m, it is not easy to pattern sub-micron features with optical lithography. Hence, we use electron-beam lithography to define nanostructures in SAW devices (Fig. 3.3(c)). To minimise the cost of electron-beam lithography, we only pattern parts of the gates with electron-beam lithography, and for the rest, we use optical lithography. In our devices, we evaporate Ti/Au for the electron-beam features first and then follow by the optical features to make sure the contact between them is functional (Fig. 3.3(d)).

Before the electron-beam lithography, a double layer of polymethyl methacrylate (PMMA) is coated on the chip. The first layer is a solution of A6 100K PMMA in anisole in a ratio 1:1 spun at 3000 rpm for 50 s. The chip, with the first layer PMMA, is then baked on a hotplate at 180°C for 3 min. Before coating the second layer, we check the first layer of PMMA under a microscope to see whether there are bubbles or defects in the layer. Next, the second layer, a solution of A11 950K PMMA in MIBK in a ratio of 1:5, is spun at 8000 rpm for 50 s, and then baked for 4 mins on a hotplate at 180°C. To obtain a clear double layer and avoid the dislocation, we spin the second layer as soon as possible when the PMMA drops cover the chip. After electron-beam lithography (written by Mr Thomas Mitchell and Dr Jonathan Griffiths), we develop the patterns in a ‘fine-structure’ developer, in which has MIBK: IPA: MEK in a ratio of 5:15:1 for 5 s. The quality of the sub-micron patterns is assessed using a microscope with a 100 times magnification. To protect electron-beam features, we directly place the chip in an evaporator and 7 nm Ti and 10 nm Au are deposited without HCl etching and plasma ashing. During Ti evaporation, the current is increased faster than in normal evaporations to minimise heating, which may melt the PMMA layer and damage the developed electron-beam
Section 3.2. Device fabrication and characterisation

Figure 3.3: Device patterns with mesa, Ohmic contacts, surface gates and IDTs.

features. After evaporation, we soak the chip in acetone overnight and use pipette agitation to achieve a good lift-off, which may take an hour or even longer. Here the use of the ultrasonic bath is dangerous: the strong vibration may loosen the contact between the GaAs substrate and the metal. To generate a 3 GHz SAW, we pattern IDTs with 250 nm finger width and gaps using electron-beam lithography together with nano-scale gates. The metal is kept thin (7/10 nm Ti/Au) to reduce the mass-loading effect from the IDTs and help to improve SAW generation.

Once electron-beam surface gates and IDTs are completed, the optical parts of surface gates are transferred using optical lithography (Fig. 3.3(d)). Here we use a double-layer photoresist to create clear undercuts for lift-off. The lift-off photoresist (LOR5B) is coated on the chip by spinning at 7000 rpm for 30 s and baking for 10 min on a 180°C hot plate. A thin photoresist S1805 is then coated on the chip by spinning at 5500 rpm for 30 s and baking for 1 min at 115°C. After alignment with Ohmic contacts and electron-beam gates, we expose the chip to UV light for 3.5 s. Because the LOR5B is more sensitive to the MF319 developer than other photoresists, only 10-20 s developing time is enough. Under a microscope, the colour difference at the pattern edge usually shows a good undercut. We perform plasma ashing and HCl dipping before evaporation. At a pressure lower than $2 \times 10^{-7}$ mbar, 20 nm Ti is deposited to create a strong Schottky barrier. Then a 100 nm-thick gold layer is evaporated. To ensure good metal adhesion especially for the bonding pads, the first few nm of Ti and Au is evaporated at a slow rate of 0.2 nm s$^{-1}$. Different to electron-beam gates, optic gates are large enough so over-heating is not a problem here. After metallisation, lift-off is achieved by soaking the chip in a solvent SVC-14 at 70°C for 10 mins. After checking the patterns, the chip is cleaned with acetone and IPA and dried with N$_2$. This evaporation process is important for bonding the
chip into the package. If the thickness of contact metal is not sufficient, it can be easily pulled off in the bonding. Poor adhesion between the metal and the substrate may also cause the same trouble.

### 3.2.4 Packaging

![Sample Holders](image)

Figure 3.4: Two types of sample holders: a coffin-style holder (a) and a CPW holder (b). In the coffin-style holder, the device is bonded to a base (1) with RF SMA connectors, then sealed with two metal lids (2 and 3). In the CPW holder, we bond the device to a base (1) with RF SMP connectors. There is only one lid (2) for the device, 2' is a lid designed for optical measurements. The arrow shows the coplanar waveguide.

Before measurements, the chip is cleaved into individual devices and bonded to a SAW sample holder. We use a diamond-tipped scriber to draw trenches between devices. During cleaving, debris may leave scratches on the surface and affect SAW propagation. To avoid this, we coat a thin layer of photoresist S1805 on the chip to protect the surface. After cleaving, each device is cleaned with acetone and IPA and mounted in a SAW sample holder with GE vanish. Then the device is bonded to the holder using a wedge bonder.

In device fabricating and packaging, bonding is one of the most dangerous processes, especially for electron-beam gates. During bonding, unpredictable electrostatic discharges may damage electron-beam gates. Therefore several protections are used during the bonding process against electrostatic discharges: 1) careful grounding by wearing an antistatic wrist strap and grounding Conan connectors that are wired to the bonding pads; 2) an ionising fan continually blowing ionised air above the device; 3) a proper bonding order with the first bond on the holder and the second bond on the device. Once the device is bonded, proper grounding is always needed.

Figure 3.4 demonstrates two types of SAW sample holders. One is a coffin-style sample holder, and the other is a coplanar-waveguide (CPW) sample holder. In the CPW sample holder (Fig. 3.4(b)), we design a coplanar waveguide to improve transmission efficiency by matching circuit impedance to 50Ω. With this holder, the
device is mounted face-up in the probe, which is suitable for optical measurements. The coffin-style sample holder (Fig. 3.4(a)) shows better grounding and sealing, giving less electromagnetic crosstalk. In our transport measurements, we use the coffin-style sample holder to minimise electromagnetic crosstalk, which shows better results than the CPW sample holder. In device packaging using a coffin-style sample holder, we solder the RF wires to SMA connectors. Here the use of solder flux is dangerous and should be avoided, because the flux may flow to the IDT and heavily damp the SAW generation.

3.2.5 Characterisation of IDTs

Figure 3.5: Scanning electron micrograph of the IDT fingers for a 1 µm SAW.

After IDT metallisation, the quality of fingers can be assessed using microscopy or scanning electron micrographs. Figure 3.5 shows an example of IDT fingers with a SAW wavelength of 1 µm. To evaluate the SAW generation, we use a two-port network analyser to measure the scattering parameters (S-parameter). By inputting an RF signal from Port 1, the reflection loss, $S_{11}$, is deduced from the reflected signal detected from Port 1. The insertion loss, $S_{12}$, is obtained from the transmitted signal detected from Port 2 (as with $S_{22}$ and $S_{21}$).

$$S_{12} = 10 \log_{10} \frac{P_{\text{transmission}}}{P_{\text{input}}}$$  \hspace{1cm} (3.9a)

$$S_{11} = 10 \log_{10} \frac{P_{\text{reflection}}}{P_{\text{input}}}$$  \hspace{1cm} (3.9b)

Firstly $S_{11}$ and $S_{22}$ are measured to check the RF signal transfer from coaxial cables to IDTs. At 2.6 GHz, both $S_{11}$ and $S_{22}$ are $\sim -3$ dB, and they are stable until the frequency reaches $\sim 2.7$ GHz. At this point a small dip appears in both $S_{11}$ and $S_{22}$, reaching $\sim -5$ dB. We explain this dip (as seen in Fig. 3.6(a)) as the power dissipated in SAW generation at the resonant frequency. For different SAW devices, the resonant frequency is slightly different, which comes from the IDT lithography and evaporation errors.

For $S_{12}$ measurement, off resonance there are no SAWs generated, and the background signal is $\sim -80$ to $-90$ dB. At the resonant frequency, SAWs are generated and received by the other IDT, observing a clear peak of $\sim -55$ dB at $\sim 2.7$ GHz (as seen in Fig. 3.6(b)). From $S_{12}$ peak the quality of SAW generation is assessed, and
Figure 3.6: Reflection loss $S_{11}$ (a) and insertion loss $S_{12}$ of devices in the CPW sample holder (b) and the coffin-style sample holder (c). The measurements are performed at an RF power of 10 dBm and $T = 4$ K.
the background signal of $S_{12}$ indicates the direct electromagnetic coupling between two IDTs. To sum up, the quality of the SAW can be roughly assessed by the ratio of these two parameters. On the main $S_{12}$ peak, a small oscillation with a period of 3 MHz is observed. This oscillation comes from a resonance between SAWs and electromagnetic waves. Due to the different propagating speed of SAWs and the electromagnetic waves, the resonant frequency is determined using Eqn. 3.10

$$f = \frac{D(V_L - V_S)}{V_L V_S},$$

where $V_L$ is $3 \times 10^8 \text{ms}^{-1}$ and $V_S$ is $3 \times 10^4 \text{ms}^{-1}$, and $D$ is the distance between two sets of IDTs. Furthermore, we observe a sudden drop after the centre resonant frequency. This asymmetry in $S_{12}$ is not fully understood. Figs. 3.6(b) and (c) show $S_{12}$ measurement in different sample holders. Good screening and sealing in the coffin-style sample holder contribute to a low $S_{12}$ background and weak electromagnetic resonance.

### 3.2.6 Characterisation of Ohmic contacts and gates

We first assess Ohmic contacts at room temperature using a probe in the cleanroom. The 2DEG resistance between two Ohmic contacts is roughly tens of kΩ. The sample holder is mounted on a 4 K probe and inserted into a LHe dewar to check the Ohmic contacts and gates. Figure 3.8(a) illustrates the measurement circuit of a SAW device. A low-noise pre-amplifier (Stanford Research Systems Model SR570) is connected to one of the Ohmic contacts, and another Ohmic contact is grounded with a BNC grounding plug. When a small DC bias of about 1 meV is applied, the current is measured with the preamp (sensitivity from 1 pA V$^{-1}$ to 1 mA V$^{-1}$) and an electrometer (Keithley 6514 system electrometer). From the bias and the source-drain current, the resistance of the 2DEG at 4.2 K is calculated, around 1 kΩ, which includes the contact resistance and a built-in resistor in the pre-amplifier (from 0 to 1 MΩ depending on the sensitivity). We repeat the same tests for other Ohmic contacts.

![Image of graph](image-url)

**Figure 3.7:** Pinch-off characterisation of a 1D channel with length $L = 1.5 \mu \text{m}$. The arrows show the voltage at gate definition and pinch-off.
After Ohmic contacts, we check the gates in a similar way. All Ohmic contacts are grounded with BNC grounding plugs, and a small bias is applied to a gate. If there is a current reading from the electrometer, this indicates a leakage current through the gate to the 2DEG. If this occurs, we need to check the device package and measurement circuit for shorts. We then sweep voltages on the split gates, $V_{SG}$, from 0 V to $-1$ V using DC voltage source (Yokogawa GS200) to characterise a 1D channel, as shown in Fig. 3.7. Between $V_{SG} = -0.2$ and $-0.3$ V, a steep decrease indicates that a large area of 2DEG below the gates has become depleted, defining a 1D channel. This voltage is termed as the definition voltage. As $V_{SG}$ becomes more negative, the 2DEG between the gates become depleted, completely at the pinch-off voltage, $V_P$. If split gates are blown up by electrostatic discharges, the 1D channel cannot be pinched off or requires more negative voltage to pinch off. In the following measurements we use the bias cool-down technique to minimise the telegraphy noise. In the biased cool-down, we apply $+0.2$ V to the split gates at room temperature. After cooling down, frozen charges induce electric fields in the donor layers by this voltage act as a gate, giving an offset in $V_{SG}$ ($-0.2$ V) at a low temperature.

3.3 SAW-driven quantised current

In a SAW electron transport measurement, the quantised current is one of the most important features. To observe it, we apply an RF signal using an Agilent analogue signal generator N5171B. Because of a long coaxial cable in the 4 K probe, the attenuation of the RF signal at 3 GHz is around 3 dB. Here, we quote the SAW power after allowing for the cable attenuation. We set $V_{SG}$ at $-0.1$ V beyond $V_P$, and sweep the frequency from 2.5 to 3 GHz at a power of 7 dBm. As the frequency close to the resonant frequency (about 2.7 GHz), the source-drain current increases or decreases significantly, which depends on the SAW propagation direction and the source-drain current direction. When the source-drain bias is reversed, either with the bias reversed or the contacts of the BNC grounding plug and the pre-amplifier swapped, the frequency-dependent SAW current is also reversed. As well as transmission measurement, we observe the resonance between the SAW and electromagnetic waves in frequency-dependent SAW current. When $V_{SG}$ is set to
be more negative than \( V_P \), the crosstalk signal is reduced, and pure SAW-pumping current dominates. The difference in the SAW-pumping current and crosstalk signal is more distinguishable in a time-resolved optical measurement of a later induced np junction.\footnote{1} From these measurements, we chose the SAW resonant frequency for the following measurements. Because of mass-loading, when the probe is lowered and the device is immersed into liquid helium, the frequency-dependent SAW current is highly damped. When we raise the probe above the liquid, the SAW current recovers again.

At the SAW resonant frequency, with a power of 7 dBm, we sweep \( V_{SG} \) in a more negative direction and observe a series of plateaus matching SAW quantised plateaus at \( I = Nef \), where \( N = 1, 2, 3, \ldots \), \( f \) is the frequency and \( e \) is the elementary charge, as shown in Fig. 3.8(b). For a SAW at 2.76 GHz, the first plateau appears at 0.44 nA, and the second appears at 0.88 nA. Close to pinch-off, the plateaus become more well-defined (with better plateau flatness). Here we use several techniques to manipulate SAW quantised pumping.

![Figure 3.9: \( dI/dV_{SG} \) as a function of \( V_{SG} \) at different RF powers from \(-3\) dBm to 11 dBm. Inset: SAW-pumping current at different powers from \(-3\) dBm to 11 dBm.](image)

1. Figure 3.9 demonstrates the power-dependence of SAW quantised plateaus. As the RF power is incremented from \(-3\) dBm to 11 dBm, \( V_P \) is shifted by up to 200 mV. At a low RF power, the SAW quantised plateaus are not well defined, misaligning with \( I = Nef \). As the RF power increases, the quantisation becomes better defined, which contributes to an improvement in the SAW amplitude with a high RF power. As the power further increases above 7 dBm, quantisation is damped, and the plateaus weaken and disappear. In the past, this has been explained as a consequence of strong heating or a crosstalk effect, which increases errors in quantisation.\footnote{2} However, we find that this is not the reason, since as the RF power rises above 10 dBm, the SAW quantised plateaus reappear and flatten again. We explain this effect as being a consequence of randomly-distributed impurities in the SAW channel (more details will be discussed in Chapter 4).

2. To improve SAW quantisation, we can apply an asymmetric bias to the split
gate, to shift the position of the SAW channel away from the centre of the split gates. The shift in the SAW channel can move away from impurities and may improve the SAW-driven quantisation.

3. We have also found that the device dimensions are very important for SAW quantisation. When comparing the SAW quantisation using different SAW channels with $L = 0.7\,\mu m$ and $1.5\,\mu m$, with the same width $W = 0.7\,\mu m$. It is easier to observe SAW-driven quantised current in the long channel ($L = 1.5\,\mu m$) than in the short one ($L = 0.7\,\mu m$). We explain this effect by the fact that if $L$ is only a little longer than $\lambda/2$, where $\lambda$ is the SAW wavelength, it may cause forward tunnelling for the electron in the SAW minimum (as introduced in Chapter 2), causing errors in quantisation.

4. We deposit a front gate at the entrance of a SAW channel. When applying a small voltage to the gate, $V_f$, we modulate the potential at the SAW entrance. Figure 3.10 shows SAW-driven quantisation at different $V_f$ from $-0.2\,V$ to $0.14\,V$ with an increment of $0.02\,V$. Inset: schematic diagram of the device with the front gate at the SAW entrance. The lines are shifted horizontally for clarity.

5. Different to the gate-defined charge-pumping, as shown in Fig. 3.1, the quan-
tised plateaus in the SAW pumping are significantly smear out when a strong perpendicular magnetic field is applied.\textsuperscript{26} Figure 3.11 shows that the SAW quantised current evolves with the magnetic field. When the magnetic field is above 0.4 T, the quantised plateaus disappear. However, we find that the pumping current significantly increases, even without quantisation, as shown in the inset of Fig. 3.11. The increase in pumping current is probably because the magnetic field gives strong confinement to the electrons in the DQDs. The back tunnelling of the electrons is highly suppressed,\textsuperscript{103} and hence the pumping current gets higher as the magnetic field increases.

![Figure 3.11: Quantised SAW current at different magnetic fields from 0 to 0.4 T. Inset: SAW current as a function magnetic field up to 1 T at $V_{\text{SG}} = -0.87$ V.](image)

### 3.3.1 Transmission model

In order to explain SAW quantised current, we use a model in which electrons in SAW minima are able to tunnel out via a saddle-point potential barrier. The transmission probability through such a barrier with potential $V(x, y) = V_0 - \frac{1}{2} m^* \omega_x^2 x + \frac{1}{2} m^* \omega_y^2 y$ is

$$T = \frac{1}{1 + e^{-\epsilon}}$$

(3.11)

where

$$\epsilon = \frac{2(E_N - \frac{1}{2} \hbar \omega_y - V_0)}{\hbar \omega_x},$$

(3.12)

and $m^*$ is the effective mass.\textsuperscript{85,86} We superpose a SAW potential on to the electrostatic potential and calculate $\omega_x$ for the barriers, together with the energy of the $N^{\text{th}}$ electron, $E_N$, which is estimated from the electron ground-state energy in the SAW minimum. A realistic electrostatic potential is calculated using Nextnano, as introduced in Chapter 2. The inset of Fig. 3.12 shows that $\omega_y$ is weakly dependent on the SAW phase, or the position in a SAW channel. Therefore we take $\hbar \omega_y$ as a
constant around 2.5 meV. In the model, we fit the SAW minimum to a parabolic potential and deduce $\omega_x$, as shown in the inset of Fig. 3.12. In this model, we take $\omega_x$ same for the tunnelling barrier.

Figure 3.12: Electrostatic profile of a 1D channel (red line) with SAW potential with an amplitude of 23 meV at different phases (black lines). Blue dots show the energy at the bottom of the SAW minimum, $E_{bm}$, at different phases. Red dots are the energy of the height of the tunnelling barrier, $E_{br}$, at different phases. Inset: Calculated $\omega_x$ and $\omega_y$ at different phases.

In the SAW pumping process, we compare the energy difference at the bottom of SAW minimum, $E_{bm}$, and the tunnelling barrier, $E_{br}$, as shown in Fig. 3.12. The energy difference determines the number of electrons and the tunnelling rates. Initially, $E_{bm}$ is much lower than $E_{br}$, so the SAW minimum can hold several electrons. As the SAW propagates, $E_{bm}$ rises more quickly than $E_{br}$ so that the difference between $E_{bm}$ and $E_{br}$ becomes smaller, and electrons with different energies tunnel out through the barrier with different probabilities. When the SAW travels to a position with a maximum gradient of the SAW channel, the difference between $E_{bm}$ and $E_{br}$ reaches a minimum, and after that maximum gradient of the 1D channel, the difference increases again. At the maximum gradient, if $E_{bm} < E_{br}$, the electron can remain in the SAW minimum and travel along the channel. If not, the electron can tunnel out through the back barrier and no such electrons can travel across the SAW channel. It is, therefore, this energy difference that determines how many electrons can travel across the SAW channel. This energy difference is controlled by the SAW amplitude and the SAW channel potential. In this experiment, we can observe the SAW quantisation by varying the SAW power or $V_{SG}$.

Confinement from both the split gates and the SAWs defines a dynamic quantum dot. Inside the quantum dot, the electron energy is quantised into discrete states. The total energy of a dot containing $N$ electrons is

$$U(N) = \sum_{i=1}^{N} E_i + \frac{(-eN + C_gV_{SG})^2}{2C},$$  \hspace{1cm} (3.13)$$

where $E_i$ is the electron energy in $i^{th}$ state, $C_g$ is the capacitance between the dot and the gate, and $C$ is the total capacitance. when one electron is added to a dot
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with $N$ electrons, the electrochemical potential changes by

$$\mu_{N+1} - \mu_N = E_{N+1} - E_N + \frac{e^2}{C}. \quad (3.14)$$

Here, the quantum-dot charging energy is $E_C = e^2/C$. The quantum dot capacitance consists of the self-capacitance of the dot, $C_{self}$, the capacitance to the surface gates $C_g$, and the capacitance in other environments, such as the source, drain, or other dots. The self-capacitance of the dot can be estimated from the capacitance of a charging disc. The other two parts are difficult to predict, especially for the SAW-driven dynamic quantum dots.

Here the saddle-point transmission model is calibrated with a magnetic field, having been calculated by Fertig and Halperin. With a definition $\Omega^2 = \omega_c^2 + \omega_y^2 - \omega_x^2$, where $\omega_c$ is the cyclotron frequency $eB/m^*$, the transmission probability Eqn. 3.11 is modified with

$$\varepsilon_N = \frac{E_N - \frac{1}{2}E_2 - V}{E_1} \quad (3.15)$$

with

$$E_1 = \frac{\hbar}{2 \sqrt{2}} \left[ (\Omega^4 + 4\omega_x^2\omega_y^2)^{1/2} - \Omega^2 \right]^{1/2} \quad (3.16)$$

and

$$E_2 = \frac{\hbar}{\sqrt{2}} \left[ (\Omega^4 + 4\omega_x^2\omega_y^2)^{1/2} + \Omega^2 \right]^{1/2}. \quad (3.17)$$

This model shows the improvement in quantisation as the magnetic field increases, which accords with the experiment with charge pumping at a low frequency. However, this model fails to explain the non-adiabatic effect on the accuracy of the quantisation of acoustoelectric current. Figure 3.1(g) shows the charge pump at 1 GHz as a function of magnetic fields. The quantisation gets worse when the magnetic field increases up to 6 T and then the quantisation of the acoustoelectric current recovers. From Eqn. 3.6, the non-adiabatic effect is determined by a factor $E_c/kT_{eff}$, where $T_{eff}$ is from Eqn. 3.7. By introducing this factor to the transmission model, we modify Eqn. 3.15 with a non-adiabatic factor:

$$\varepsilon_N = \frac{E_N - \frac{1}{2}E_2 - V}{E_1} \cdot \left( \frac{E_c}{kT_{eff}} \right). \quad (3.18)$$

By introducing this factor, we can model the SAW quantised current in different magnetic fields at a base temperature of $T = 2$ K. At around 0.5 T, the quantisation of the SAW acoustoelectric current degrades, and at around 1 T, the quantisation disappears, which approximately matches the experimental result. However, the non-adiabatic excitation transition peaks are not observed. In a high-frequency gate-defined charge pump, as shown in Fig. 3.1(g), quantisation initially gets worse and then improves for a high field. This recovery happens because the confinement becomes strong enough, and the non-adiabatic error is overcome. However, in our SAW-pumping, this is not observed. We applied a magnetic field up to 7 T, and there was still no sign of a recovery in quantisation.
3.4 SAW-pumping spectroscopy

As has been introduced above, electron energy inside a dynamic quantum dot is important for the SAW quantisation, and the energy difference between the \( N \)th and \( (N+1) \)th electron will determine the flatness of the \( N \)th plateau. In a static quantum dot, we sweep the DC bias and measure the addition energy from the Coulomb blockade diamonds. However, in a dynamic quantum dot, it is not straightforward to measure this addition energy in the quantum dot. Therefore we have designed a spectroscopy device to measure electron energies of a SAW-driven dynamic quantum dot.

Figure 3.13: Modelled quantisation with transmission model from \( B = 0 - 1 \) T with different \( l \) and \( T \) from the SAW phase from 0.45 to 0.6. The lines are shifted horizontally by clarity. Inset: Wave-functions in a parabolic potential at different magnetic fields.

Figure 3.14: Schematic diagram of a SAW spectroscopy device. There is a SAW channel defined by split gates, an emitter, screening gates, and a spectrometer.
The device consists of a pair of split gates, an emitter, a pair of screening gates and a spectrometer, as shown in Fig. 3.14. Negative voltages are applied to split gates, $V_{SG}$, and deplete electrons beneath gates, defining a SAW channel. At the edge of the SAW channel, the SAW collects electrons from the reservoir and confines them in SAW minima. As the SAW passes through the SAW channel, the longitudinal confinement by the SAW shrinks the minima and pushes electrons out of SAW minima and back to the reservoir. The quantised SAW-driven current is measured by low-noise current pre-amplifiers. As $V_{SG}$ becomes more negative, the SAW pumping current is pinched off. This quantised current clearly demonstrates the formation of dynamic quantum dots with a fixed number of electrons ($N = 1, 2, 3, \cdots$). Once DQDs are defined, by applying a negative bias on the emitter gate, $V_E$, a thin barrier is raised, re-modulating the DQDs and pushing electrons out with finite kinetic energy. These hot electrons travel along a screened channel ($V_{SC}$ on screening gates) for 3 $\mu$m and reach the other barrier. The height of the barrier is controlled by the voltage on the spectrometer ($V_S$). With a spectrometer, the energy spectroscopy of SAW-driven DQDs is carried out.

3.4.1 Manipulation of SAW-driven DQDs

Figure 3.15(a) shows a potential hill along a SAW channel by applying $V_{SG}$ to a pair of split gates. When the SAW reaches the edge of the potential barrier (position 1), the electron density decreases and thus electron screening of the SAW potential is strongly suppressed. The SAW then collects electrons in each minimum and begins to climb the potential hill. As the SAW continues to propagate, the size of dot becomes smaller and forms a DQD. When the DQD reaches position 2, electron depopulation is highly suppressed, and the number of electrons in each DQD become fixed. Even with a set number of electrons, the electron energy ($E_e$) in the DQD increases as the SAW climbs the potential hill, reaching a maximum at the peak of the potential hill (position 3). In the downhill part of the SAW channel, the above process is reversed. Finally, the electron in the DQD returns to the Fermi sea on the right.

In this standard SAW-pumping process, it is difficult to probe the electron energy inside a SAW-driven DQD. We introduce an extra potential barrier in the downhill part of the SAW channel to manipulate the DQD. As shown in Fig. 3.15(b), the emitter gate creates a sharp barrier to manage the DQD relaxation process. When the SAW-driven DQD comes across the emitter barrier, it is re-modulated. Electrons with higher energy are pushed out of the SAW-driven DQD again, and the electrons left behind can tunnel out through the emitter barrier with finite kinetic energy. Therefore, the barrier can emit hot electrons with finite electron energy, as shown in positions 2-4 in Fig. 3.15(b).

Figure 3.16 shows $|\nabla I_{SAW}| = |\partial^2 I_{SAW}/\partial V_{SG} \partial V_E|$ as a function of $V_{SG}$ and $V_E$, and demonstrates the manipulation of SAW-driven DQDs. Once the SAWs initialise the quantum dot in the uphill part of the SAW channel, the SAW minimum is re-modulated in the downhill part of the SAW channel. For example, when a DQD is initialised with two electrons in the SAW channel ($2e_f$) are re-modulated, one of the electrons is thrown back to the Fermi sea, and the other electron tunnels through the emitter barrier with finite kinetic energy and travels ballistically towards the
Figure 3.15: (a) SAW-pumping process across a SAW channel (black lines). At position 1, two electrons are trapped in the SAW minimum. Then, at position 2, one electron is pushed out, and the other electron remains in the minimum. As the SAW propagates to positions 3 and 4, the electron remains in the minimum. After position 5, the electron returns to the Fermi sea (red region). (b) SAW-pumping process with a SAW channel and an emitter barrier. At position 1, the DQD start with 2 electrons. As the SAW propagates, the second electron at energy $\mu_2$ tunnels through the barrier with kinetic energy $E_2$ above the 2DEG Fermi energy, $E_F$. Later, the last electron at energy $\mu_1$ tunnels through the barrier with kinetic energy $E_1$. Inset: Schematic diagram of a SAW channel with an emitter.

spectrometer ($e_f$). The emitter gate is important in this experiment. By measuring the electron kinetic energy, we can carry out the energy spectroscopy of the DQD.

3.4.2 Electron energy distribution

A SAW is a propagating wave with a specific direction. The measured current is related to the electron flow direction. Here we define the electrons flowing into the current pre-amplifier as a negative current. SAWs can pump electrons across the potential barrier, and the possibility of pumping depends on the maximum slope of the potential barrier. In this case, SAWs can also pump electrons from the 2DEG (positive current in $I_2$) directly across the spectrometer (negative current in $I_3$). This negative current may be confused with hot electrons tunnelling from SAW-driven DQDs. We narrow the metallic surface gate down to 100 nm to increase the
maximum slope of the spectrometer and suppress this direct pumping across the spectrometer. Experimentally, we can measure this pumping current directly across the spectrometer. Due to the narrow gate, the SAW-pumping current is cut off at around $V_S = -0.3 \, \text{V}$. Therefore we set the spectrometer high enough, $V_S < -0.4 \, \text{V}$, to exclude this direct pumping current across the spectrometer and to make sure the electrons measured in $I_3$ are from the SAW-driven DQDs.

Figure 3.17(a) demonstrates the SAW-driven quantised current as a function of $V_{SG}$ and $V_S$. When $V_S$ is less negative ($V_S = -0.4 \, \text{V}$), or the spectrometer barrier is not high enough, hot electrons travel through the screening channel and pass the spectrometer and are detected as $I_3$. If $V_S$ becomes more negative, reaching $-0.6 \, \text{V}$, the spectrometer barrier becomes higher. The hot electrons fail to pass through the spectrometer and are reflected to the cold Fermi sea, measured in $I_2$. Figure 3.17(b) demonstrates the swapping of $I_2$ and $I_3$ when sweeping $V_S$ at the first plateau of quantised current. We calibrate the spectrometer and convert voltage $V_S$ into energy $E_S$. Experimentally, the spectrometer is calibrated using similar experimental methods.\(^{105,106}\) Instead of using a SAW, the source bias, $V_{SD}$, increases and ejects hot electrons over the channel with a finite kinetic energy of $E_F + e|V_{SD}|$, where $E_F$ is the Fermi level. By sweeping $V_S$ and $V_{SD}$, the spectrometer voltage can be converted to the electron energy, in our device $E_S = (-0.33 \times V_S - 0.15) \cdot e$. Theoretically, we calculate the electrostatic profile at different $V_S$ with improved boundary conditions in a self-consistent electrostatic Poisson solver (as discussed in Chapter 2). The spectrometer height is $E_S = (-0.3 \times V_S - 0.12) \cdot e$, which matches the experimental results. After spectrometer calibration, the full width at half maximum (FWHM) of the single-electron wave-packet is around 8 meV, as shown in the inset of Fig. 3.17(b).

Figures 3.18(a) and (b) show grey-scale plots of $|\nabla I| = |\partial^2 I/\partial V_{SG} \partial V_S|$ in $I_2$ and $I_3$ as a function of $V_{SG}$ and $V_S$. It is clear that SAW-driven DQDs evolve with a fixed number of electrons $N = 1, 2, 3, \ldots$. There is a clear boundary in the
Chapter 3. Energy spectroscopy of SAW-driven quantum dots

Figure 3.17: (a): Quantised SAW current $I_2$ and $I_3$ at $V_S = -0.4$ V and $-0.6$ V. (b) Acoustoelectric current ($I_1$, $I_2$ and $I_3$) as a function of $V_S$. Inset: $dI_3/dV_S$ as a function of $E_S$, which is converted from $V_S$.

transition between $I_2$ and $I_3$. Fig. 3.18(c) shows the transition point between $I_2$ and $I_3$ (as red dots in Fig. 3.18(a)) as a function of $V_{SG}$. It marks the minimum electron energy of the hot electron tunnelling out of the SAW-driven DQDs. Using the spectrometer, we have evaluated the energy spectroscopy of SAW-driven DQDs. Fig. 3.18 (c) shows the energy spectrum of a DQD, the last electron in the DQD having the highest energy of 55 meV. As the number of electrons increases, the minimum electron energy decreases to around 38 meV for the DQDs with 5 electrons. The energy difference is around 3 meV, and the difference becomes smaller when more electrons fill the quantum dot. This energy difference is not the classical addition energy in static quantum dots. It is the energy difference marked $E_1 - E_2$ in the inset of Fig. 3.15(b). In previous measurements, Astley et al. observed electrons tunnelling from the DQDs. From the tunnelling probability of different plateaus, they calculate the energy difference, which around 3 meV and similar to our measurements. Fletcher et al. used a similar spectrometer to investigate single-electron wave-packet in a DQD. By sweeping the spectrometer, the quantised electron energy was observed. However, we do not observe the quantised electron energy in SAW DQDs when sweeping $V_S$. This is probably because the FWHM of
Figure 3.18: Grey-scale map of $|\nabla I| = |\frac{\partial^2 I}{\partial V_{SG} \partial V_S}|$ in $I_2$ (a) and $I_3$ (b) as a function of $V_{SG}$ and $V_S$. (c) Spectroscopy of minimum energy of the electron wave packet (red), and measured energy of electrons with DQDs with $N^{th}$ electrons (black).

energy spectrum of the single electron DQD (8 meV from the inset of Fig. 3.17(b)) is greater than the addition energy of the DQD (around 3 meV).

### 3.4.3 Suppression of electron-electron interactions

In Figure 3.14, an empty channel is created by applying a voltage to the screening gates, $V_{SC}$. Figure 3.19(a) demonstrates the importance of screening gates. Without screening gates, $V_{SC} = 0$, electrons with fixed kinetic energy fail to travel over 3 $\mu$m, contributing to $I_2$. When $V_{SC} = -0.44$ V, the electrons are depleted and create an empty channel. Electrons can travel to the spectrometer and are measured. Theoretically, electrons with kinetic energy (hot electrons) interact with electrons in the Fermi sea (cold electrons), and cool down and relax to the Fermi sea. In Landau-Fermi liquid theory, the scattering length of hot electrons, $l_{e-e}$, strongly depends on the kinetic energy. $l_{e-e}$ of hot electrons with kinetic energy of 60 meV...
is about 400 nm, which is much smaller than the device dimension.\textsuperscript{105} This explains why the hot electrons cannot reach the spectrometer.

To suppress the strong electron-electron interaction, we create an empty channel for hot electrons moving towards the spectrometer by using screening gates. Hot electrons relax due to electron-electron interaction. However, even in absence of such scattering, they can emit longitudinal optic (LO) phonons provided that the wavefunction is initialised and find states to overlap in space. In the GaAs, the LO phonon has an energy of 36 meV, which has been observed in previous research.\textsuperscript{105,107} Figure 3.19 (b) shows the emission of LO phonons in this measurement. The two peaks are separated with a 0.1 V shift in $V_S$, which indicates the energy difference is around 34 meV, matching the LO phonon energy in the GaAs. As $V_{SC}$ becomes further negative, the emission of LO phonons is suppressed.

![Figure 3.19: (a) Quantised SAW current $I_2$ and $I_3$ at different screening gate voltage $V_{SC} = -0.44$ V and 0. (b) Energy spectrum of $I_3$ and its differential. The energy difference between the two peaks is $\sim 34$ meV, comparable to $\hbar \omega_{LO} = 36$ meV.](image)

Alternatively, a strong out-of-plane magnetic field can suppress electron-electron interaction to increase $l_{e-e}$. Taubert \textit{et al.} have studied the electron-electron scattering with and without a magnetic field.\textsuperscript{105} In the calculation $l_{e-e}$ for hot electrons with energy of 60 meV increases to 2 $\mu$m at an external magnetic field of 5.6 T. Fletcher \textit{et al.} suppressed the electron-electron interaction using a strong out-plane magnetic field (12 T).\textsuperscript{97} Experimentally, we apply a strong out-of-plane magnetic field to the SAW-driven DQDs to suppress electron-electron interaction. As we increase the magnetic field, the SAW-pumping current begins to increase significantly,
but the quantisation of SAW-pumping disappears when the magnetic field is greater than 0.5 T, which was discussed in the previous section. Therefore, we prefer to using the screening gates to suppress the electron-electron interaction.

3.5 Spectroscopy of SAW-ejected electrons

![Figure 3.20](image)

Figure 3.20: (a) Schematic diagram of the spectroscopy device with screening gates for SAW-ejected electrons. There is a SAW channel defined by split gates, screening gates, and a spectrometer. (b) Schematic diagram of the electrons ejected from the dynamic quantum dot (blue blob). The SAW is propagating from right to left.

In the formation of SAW-driven DQDs, some electrons are dragged by the SAW to high energy, but then are ejected back to the reservoir as the dot is squeezed, as shown in Fig. 3.20(b). To investigate the ejected electrons, we reverse the SAW propagation direction in a SAW spectroscopy device (as seen in Fig. 3.20(a)). SAWs collect electrons outside the SAW channel. As they pass through the SAW channel and the SAW minima shrink, the electrons are pushed out. The remaining electrons are dragged across the SAW channel and produce a quantised SAW current. Electrons ejected from the SAW minimum travel back to the spectrometer. As for the measurement in previous section, the ejected electrons move ballistically in an empty channel created by screening gates. If the ejected electrons have energy higher than the spectrometer height, $E_e > E_S$, electrons contribute to $I_3$.

From the electron flow direction, the ejected electrons contribute to negative current in $I_3$, which is opposite to the electrons directly pumped across the spectrometer. Fig. 3.21(a) shows the SAW-pumping current, $I_1$, and the SAW-ejected current, $I_3$, as a function of $V_{SG}$. $I_1$ drops and is pinched off as $V_{SG}$ decreases. Meanwhile, $I_3$ increases until $I_1$ is fully pinched off, then $I_3$ decreases. Theoretically, when the SAW-pumped current drops from $2e\bar{f}$ to $e\bar{f}$, the ejected current should increase by $e\bar{f}$. Fig. 3.21(a) shows the first plateau in the SAW-pumped current as well as a plateau in the SAW-ejected current, which gives evidence that the electrons measured in $I_3$ are electrons ejected from the SAW-driven DQDs. However, the quantisation is very poor in the SAW-pumped current. We find that the spectrometer severely damages the SAW quantisation. When $V_S = 0$, clear quantisation is observed, but when $V_S = -0.4$ V the SAW-driven current is still similar, but the quantised plateaus disappear, as seen in Fig. 3.22. The reason for this damage is
Chapter 3. Energy spectroscopy of SAW-driven quantum dots

not apparent. From the power-dependence, we conclude that this disappear of the quantisation is not because of the screening of SAW by the spectrometer gate. The direct cross-capacitance from the spectrometer to the SAW channel should to be very weak and not affect the SAW entrance, which is 3 \( \mu \)m away from the spectrometer.

![Figure 3.21](image)

Figure 3.21: (a) SAW-pumped \((I_1)\) and SAW-ejected \((I_3)\) current as a function of \(V_{SG}\). (b) Comparison of the model and experiment of the energy of ejected electrons as a function of \(V_{SG}\). Inset: SAW channel potential with different \(V_{SG}\) The red asterisks indicate the position at which the electron ejection occurs.

According to the SAW-pumping mechanism, the energy of ejected electrons is a function of \(V_{SG}\). Before pinch-off, the maximum slope of the SAW is larger than that of the SAW channel, \(S_{SAW}^{max} > S_{Ch}^{max}\), and the maximum electron energy increases linearly with decreasing \(V_{SG}\). At pinch-off, \(S_{SAW}^{max} = S_{Ch}^{max}\), and the last electrons are ejected with maximum energy. This position is a critical point in the SAW-pumped and ejected current, shown at the \(\alpha\) point in the inset of Fig. 3.21(b). As \(V_{SG}\) further decreases, \(S_{SAW}^{max} < S_{Ch}^{max}\), and the ejected electron energy starts to decrease. This trend matches the experimental measurements, as shown in Fig. 3.21(b). However, in these measurements, we set \(V_S\) to negative to make sure there is no crosstalk signal or other RF rectification current.\(^{108}\) In that case, the signal in \(I_3\) is much weaker than it in \(I_1\).
3.5.1 Ways of improving quantisation

In a gate-defined charge pump, the accuracy of quantisation is much better than for the SAW-driven quantised current. The dimension of the gate is as narrow as 50 nm and the confinement energy $\hbar \omega_0 = 10 \text{ meV}$, which is much stronger than the estimated SAW confinement $\hbar \omega_0 \simeq 3 \text{ meV}$. So it is likely that the strong confinement is important for improving SAW quantisation. There have been a few attempts to improve SAW quantisation:

- By increasing SAW frequency, the longitudinal confinement becomes stronger. Hence quantisation should be improved. However, a higher frequency causes stronger non-adiabatic errors, which may reduce the quantisation. Also, increasing the frequency causes the more serious EM crosstalk.

- An increase in SAW amplitude improves longitudinal confinement. However, we cannot simply increase the SAW amplitude by increasing RF power, which will cause a strong heating effect, reducing the SAW quantisation. We could increase piezoelectric coupling between the IDT and the substrate. One possible way would be to deposit a layer of ZnO to increase the SAW amplitude.

3.6 Conclusion

In this chapter, we have introduced the fabrication of SAW devices in GaAs HEMTs and discussed results of SAW quantised current with and without a magnetic field. With the transmission model, we have modelled the SAW-driven quantisation to explain why it degrades in a magnetic field with non-adiabatic errors and back-tunnelling suppressing. Then we have also investigated the energy spectroscopy of SAW-driven DQDs and found the energy difference between the first and second electrons in a DQD to be around 3 meV. Compared to the gate-defined charge pump, this small energy difference is probably the main limitation in improving the SAW quantisation.
4.1 Motivation

GaAs is not a popular material to use as a piezoelectric substrate. Other materials, such as LiNbO$_3$, AlN and ZnO, demonstrate better piezoelectric properties than GaAs. However, a GaAs/AlGaAs heterostructure exhibits excellent electronic properties with a high-mobility 2DEG. In previous SAW-pumping experiments, because of the poor piezoelectric coupling coefficient in GaAs, a high SAW power is needed to drive a quantised SAW-driven current. This strong SAW power, causing heating, increases the electron and lattice temperatures. In a cryostat, this SAW power severely diminishes the available cooling power of the condensed $^3$He and makes it difficult for the system to maintain a base temperature of 300 mK. Furthermore, a high RF power is also accompanied by a strong electromagnetic wave, which couples to gates and the pick up excites electrons and cause unpredictable effects in the system. For example, in a high-frequency charge pump, a strong rectification current has been observed from AC voltage modulation. Meanwhile, electromagnetic waves couple with SAWs and generate ripples on the SAW resonance, which accounts for the well-known crosstalk.

ZnO has been widely used in the SAW technique, and mostly, the ZnO is grown on a sapphire or SiO$_2$ substrate. In 2011 Pedrós et al. performed a detailed study of SAW-guided propagation in ZnO/GaAs systems with a thin ZnO film on a GaAs substrate. Due to the SAW velocity in ZnO is slower than it in GaAs, this slow-on-fast system shows multi-mode wave propagation, as shown in Fig. 4.1. Except for the fundamental Rayleigh mode, there are also Sezawa modes propagating in the ZnO overlayer. A Sezawa wave is a plate wave with an asymmetric mode. Becomes of the acoustic impedance mismatch, the Sezawa wave is mainly in the ZnO layer. With 1 μm-period IDTs, the Rayleigh mode appears at around 2.6 GHz. The Sezawa waves depend on a ratio of ZnO thickness and SAW wavelength. The first Sezawa mode resonant frequency decreases from 3.2 GHz to 2.8 GHz as the thickness increases from 0.98 to 2.5 μm. At a high ratio of 2.5, the second Sezawa mode is also observed. Meanwhile, the piezoelectric potential and the depth profile of particle displacement are calculated using the transfer-matrix method for both Rayleigh and Sezawa modes. Figures 4.1(e) and (f) show the simulation of the piezoelectric coupling coefficient, $K^2$, of the Rayleigh and Sezawa
mode at different depths as a function of $kH$, where $k$ is the SAW wavenumber, and $H$ is the thickness of the ZnO film. The effective piezoelectric coupling coefficient, $K_{\text{eff}}^2$, at 100 nm below the ZnO/GaAs interface is also simulated. The maximum $K_{\text{eff}}^2$ appears at $kH = 4$ with is 0.3%, which is much higher than 0.06% in GaAs. However, there are no experimental results showing an enhancement of $K_{\text{eff}}^2$ at the 2DEG.

Figure 4.1: Transmission of SAWs on ZnO/GaAs heterostructures with different ZnO thicknesses $H/\lambda = 0.98$ (a), 1.2 (b), 1.38 (c), 2.5 (d). The Rayleigh and Sezawa mode are labelled $R$ and $S_1$ or $S_2$. The piezoelectric coupling coefficient at the surface (black line), interface (black dashed line) and at 100 nm below the interface (red dashed line) of the Rayleigh-mode (e) and Sezawa-mode (f). Figures from Ref. 76.

The Sezawa mode in a ZnO/GaAs systems was also investigated and it was found that there was a lower attenuation of the Sezawa mode propagation in liquid helium. In measurements, when the device is inside the liquid helium, the SAW generation and propagation will be highly suppressed. Pedrós et al. observed that the Rayleigh mode and Sezawa mode survived inside liquid helium, and, in particular, the Sezawa mode only attenuated 10 dB below and above the liquid. For the Sezawa mode, the particle motion perpendicular to the surface is less than the Rayleigh mode. Therefore it is less affected by the mass-loading effect. In this chapter, we report the enhancement of SAW-pumping in a ZnO/GaAs/AlGaAs heterostructure. The ZnO layer is sputtered on the GaAs heterostructure to improve the SAW amplitude, and thus SAW-pumping.
4.2 Fabrication

The fabrication of a SAW device in ZnO/GaAs heterostructures is complicated and low-yield. Standard processing, involving mesa etching, Ohmic contacts, and optical and electron-beam gate evaporation, has already been introduced in Chapter 3. Here I mainly discuss the buffer-layer deposition and ZnO sputtering.

4.2.1 High-target utilisation sputtering

There are several techniques for growing a thin film ZnO, such as atomic-layer deposition (ALD), pulsed layer deposition (PLD), molecular-beam epitaxy (MBE), RF magnetron sputtering and so on. Table 4.1 shows advantages and disadvantages of each method.

<table>
<thead>
<tr>
<th>Techniques</th>
<th>Advantages</th>
<th>Disadvantages</th>
</tr>
</thead>
<tbody>
<tr>
<td>ALD</td>
<td>low defect density</td>
<td>low rate, poor crystallisation</td>
</tr>
<tr>
<td>MBE</td>
<td>high quality</td>
<td>high deposition temperature</td>
</tr>
<tr>
<td>RF magnetron</td>
<td>high deposition rate</td>
<td>high defect density</td>
</tr>
<tr>
<td>HiTUS</td>
<td>high quality</td>
<td>ion bombardment</td>
</tr>
</tbody>
</table>

Table 4.1: Comparison of ZnO deposition techniques.

For example, the ALD technique produces good quality ZnO with a low defect density. However, the ALD is only suitable for thin film deposition (less than 100 nm), and not for a thick layer. Another problem of ALD is the poor crystallisation of ZnO, which is important for SAW generation and propagation. Ideally, the growth direction should be along the c-axis for good piezoelectric properties. However, during the ALD process, the ZnO is not grown in c-axis unless the substrate is heated up to a few hundred °C and there is a particular flow of oxygen. In MBE-grown ZnO, the crystallisation is good, but the growth temperature (around 1000 °C) is too high for GaAs/AlGaAs heterostructures. Additional annealing or doping damages the electrical properties of the 2DEG. In RF magnetron sputtering, the temperature is safe for a GaAs/AlGaAs heterostructure, and the deposition rate is high enough for a thick ZnO layer to be deposited. However, the quality of ZnO grown by RF magnetron sputtering is poor with a high density of defects.

In 2010, García-Gancedo et al. developed a technique for ZnO deposition using a high target utilisations sputtering (HiTUS) system, as shown in Fig. 4.2. An RF signal generates argon plasma in a side chamber, and the plasma is then launched into the main chamber and steered to a high-purity (99.99 %) Zn target. Due to the layout of electromagnets, the plasma is not directed to the sample, avoiding the additional ion bombardment and damage to the substrate. The main chamber is evacuated to 10⁻⁶ mbar by a turbo pump. Zinc ions are deposited on the substrate and oxidised with a controlled oxygen flow. As a consequence, ZnO is also deposited at a high rate with a low density of defects at room temperature. If the power, the argon and the oxygen flow rate are controlled, ZnO deposition can be manipulated and optimised. The quality of the ZnO is firstly checked under a microscope to estimate the defect density. We then use an atomic force microscope...
Figure 4.2: Schematic diagram of the HiTUS process. Figure from Ref. 75.

(AFM) to study the morphology of the ZnO film, which is essential for SAW generation and propagation. The crystallisation of the ZnO film is assessed by X-ray diffraction (XRD) and scanning electron microscopy (SEM). The film exhibits the c-axis orientation normal to the substrate. The full width at half maximum (FWHM) of the XRD curves indicates the quality of crystalline properties.

To maximise the enhancement of SAWs at the level of the 2DEG, we deposit a thin layer of ZnO above the IDTs. In this case, the GaAs/ZnO interface is essential for SAW generation and propagation. The crystallisation of a ZnO layer at the beginning of deposition becomes critical. In previous research, we set the O₂ and Ar flow at 40 sccm, and deposited the ZnO at a rate of around 50 nm/min. In the first few iterations, we followed the usual HiTUS process for ZnO and found poor SAW generation and propagation, probably caused by the poor piezoelectric properties of ZnO at the beginning of deposition. This may be because the deposition rate is so fast that the zinc ions are not fully oxidised. Some of the devices show poor insulation, and nano-scale gates below the ZnO layer are shorted together. To deposit a high-quality ZnO film on a GaAs heterostructure to maximise the piezoelectric coupling, we optimised the HiTUS process. Firstly, we kept the sample in a dry and clean environment before the HiTUS process. Any water and dust in atmosphere
will contaminate the surface and affect the crystallisation of ZnO at the beginning of the deposition. Secondly, the deposition rate was slowed down by controlling the O\textsubscript{2} and the Ar flow rate. By increasing the O\textsubscript{2} and Ar flow rates to 55 sccm, the deposition rate is slowed down to 30 nm/min.

Figure 4.3: Scanning electron micrograph of ZnO grown by HiTUS. There is a gap at the edge of the ZnO layer and the substrate, indicated by the red rectangle.

4.2.2 Buffer layer

In a sputtering process, there may be ion implantation in the substrate. Although HiTUS will reduce the density of ion implantation as there are ions accelerated towards the substrate, it can still damage the conductance of a 2DEG in a GaAs/AlGaAs heterostructure, probably by depleting carriers. After the direct sputtering process on the GaAs/AlGaAs heterostructure, the resistance of the 2DEG between two Ohmic contacts, at around 4 K, is approximately 2 M\(\Omega\), which is a lot higher than before the HiTUS process (around hundreds of ohm). As acceptors, the zinc ions may dope the GaAs \(p\)-type during the sputtering. However, we grew ZnO on a GaAs heterostructure with a two-dimensional hole gas (2DHG) using HiTUS, and still found the damage.\textsuperscript{102} Currently, the reason for the damage has not been fully explained. In this thesis we use a GaAs/AlGaAs heterostructure with a 2DEG situating 90 nm below the surface, and this depth is not sufficient to avoid ion implantation from HiTUS. Finally, by using a buffer layer as will be described below, we do succeed in preventing damage to 2DEG conductance in the HiTUS process.

Photoresist

Before the ZnO sputtering, we spin 1.3 \(\mu\)m-thick photoresist to cover the contacts. After ZnO sputtering, we remove the ZnO above the contacts. When measuring the resistance of the 2DEG at \(T = 4\) K, we find that the resistance between two Ohmic contacts across the mesa is around 2 M\(\Omega\), and the resistance between two adjacent Ohmic contacts is around 200 \(\Omega\). This phenomenon indicates ZnO sputtering damaging the 2DEG area where it is not covered by the photoresist. This photoresist layer works as a buffer layer to prevent the damage from HiTUS process.
However, a photoresist layer is not suitable as a buffer layer. Therefore we need to develop other materials for the buffer layer. This buffer layer requires a thin film to provide proper insulation, and this is must be as thin as possible to minimise the SAW attenuation.

**ZnO by spraying**

Ideally, the buffer layer for ZnO HiTUS should also be a ZnO thin film. We firstly use a spray pyrolysis technique to grow a thin ZnO film. This was carried out by Dr. Junhee Cho in the Department of Engineering. Usually, the spray pyrolysis process needs to heat the substrate above 300°C. However, this temperature is too high for a SAW device in a GaAs/AlGaAs heterostructure. Extra annealing or doping will damage the 2DEG properties. To avoid this, we decrease the temperature to 200°C and spray a 20 nm ZnO film as a buffer layer. After the HiTUS process, we find that the damage to 2DEG conductance is prevented. However, as the temperature decreases, the quality of the sprayed ZnO film is highly degraded. There are a lot of pin-holes in the buffer layers, as shown in Fig. 4.4. In this case, a ZnO thin film using spray pyrolysis is not suitable for SAW devices. The high defect density and the rough surface probably affect SAW generation and propagation.

![Spray ZnO](image)

**Aluminium oxide**

Because of the poor quality of the sprayed ZnO thin film, we develop an Al$_2$O$_3$ buffer layer to protect 2DEG from the ZnO HiTUS process. There are two techniques for depositing Al$_2$O$_3$: one is to use electron-beam evaporation, and the other one is to use ALD.

To pattern the Al$_2$O$_3$ film, double-layer photoresist provides a clear under-cut for the lifting off process after evaporation. We mount the chip in an electron-beam evaporator and pump down to $10^{-5}$ mbar. Then oxygen gas is filled up to 5 mbar and pumped out for 3-4 cycles. Before deposition, a high-voltage electron-beam is focused on a large piece of Al$_2$O$_3$ crystal to warm up and stabilise the electron beam. When it is stabilised, the current is increased to 100 mA and the deposition rate is controlled to below 0.3 nm/s. After evaporation, the system needs to be left at least 30 mins so that the Al can be fully oxidised. During evaporation, the shutter
is set to a specific position to prevent ions accelerated by the high voltage directly impinging on the chip. Then the chip is placed in acetone for lift-off, and a few seconds in an ultrasonic bath is helpful to clear pattern edges.

As discussed above, a thin film of photoresist can protect the conductance of 2DEG during the sputtering process. We perform the same test on the SAW device with a 20 and 50 nm Al₂O₃ buffer layer using electron-beam evaporation. The 2DEG is successfully protected by the Al₂O₃ buffer layer, and there is no difference between the devices with a 20 and 50 nm Al₂O₃ buffer layer. This shows that a 20 nm-thick Al₂O₃ is able to protect the 2DEG during the HiTUS process. We also perform further tests using mesoscopic measurements in nano-scale split-gate devices. We use a device with 14 1D channels formed by 15 split gates and measure their pinch-off characteristics. For a 1D channel of length $L = 1.5 \mu m$ and width $W = 0.7 \mu m$, the pinch-off voltage is around $-0.9 \text{ V}$. After depositing an Al₂O₃ buffer layer using electron-beam evaporation and ZnO HiTUS, some of the 1D channels pinch off at $-0.25 \text{ V}$, as shown in Fig. 4.5. After the ZnO is etched away by 20% HCl, the pinch-off voltage is still around $-0.25 \text{ V}$. This test proves this damage is from the Al₂O₃ buffer layer and not the ZnO layer. This less negative pinch-off voltage indicates the split gates are shorted together through the Al₂O₃ buffer layer. During evaporation, some Al ions are not fully oxidised, causing localised poor insulation in the buffer layer.

To prevent these local defects, we improved the quality of the Al₂O₃ buffer layer using ALD. In the ALD process, the amorphous Al₂O₃ uniformly covers the mesa and the nano-scale gates. The amorphous Al₂O₃ is difficult to remove. Usually hydrofluoric (HF) acid is usually used to etch and pattern the Al₂O₃. Because the pattern of buffer layer is larger over hundreds of microns. Therefore, we use a double-layer photoresist lift-off process for the 20 nm Al₂O₃ buffer layer. We leave a 10 μm gap at the edge of the mesa to make sure the buffer layer fully covers the mesa after lift-off. With the amorphous Al₂O₃ buffer layer, the 2DEG is further protected during the HiTUS process, and the 1D channels are normally pinched off around $-1 \text{ V}$. Figure 4.6 shows the fabrication process for the SAW device in a GaAs/AlGaAs heterostructure with an Al₂O₃ buffer layer deposition using ALD and a ZnO layer using HiTUS.

4.3 Results and discussions

We have successfully deposited ZnO on a GaAs/AlGaAs heterostructure without damage to the 2DEG. We then characterise the SAW generation and propagation in
Section 4.3. Results and discussions

Figure 4.6: Schematic diagram of fabrication of the SAW device with a Al₂O₃ buffer layer and a ZnO layer.

a ZnO/GaAs heterostructure. After that, we test SAW-pumping enhancement with a ZnO overlayer. Both of these demonstrate an improvement in SAWs with a ZnO overlayer grown by HiTUS.

4.3.1 Characterisation of IDTs

Firstly, we characterise the SAW generation and propagation with a ZnO overlayer by analysing the reflection $S_{11}$ or $S_{22}$ and insertion loss $S_{12}$ or $S_{21}$ using a network analyser. GaAs and ZnO are both piezoelectric substrates. Therefore the position of the IDT needs to be chosen carefully. To maximise the SAW potential amplitude at the 2DEG, it could be worthwhile to pattern the IDT at the ZnO/GaAs interface. However, the crystallisation of ZnO at the interface may not be as good as the surface, especially on the IDTs metal. The non-uniformity in the surface morphology can influence the crystallisation. Hence the generation and propagation of SAWs may also be influenced.

Figure 4.7 compares the transmission $S_{12}$ in three devices with IDTs on a GaAs substrate, at the GaAs and ZnO interface, and on the ZnO surface. To simplify the fabrication, we use 4 $\mu$m SAWs with optical lithography instead of 1 $\mu$m SAWs with electron-beam lithography. The 4 $\mu$m SAWs have a metal finger width of 1 $\mu$m and separation of 1 $\mu$m. This dimension is close to the extreme of optical lithography. Hence we use double-layer photoresist for clear under-cuts. The edge-bead effect in the spinning process causes uneven photoresist at the edge of the chip, which reduces the accuracy of optical lithography. Therefore, an edge-bead-removing process is necessary to provide good contact between mask and chip for the high-resolution lithography. For successful fabrication of SAW transducers, the precise exposure and developing time are essential. After several attempts, we optimised the exposure time to be 3.2 s and developing time to be 10 s. When depositing IDTs on a pure GaAs substrate, as shown in Fig. 4.7(c), we observe the $S_{12}$ peak at only $-90$ dB at a SAW resonant frequency of 730 MHz.

Here the GaAs substrate is a pure GaAs substrate before MBE growth. After
1 µm ZnO is deposited, the resonant frequency shifts to around 470 MHz. This shift is because the SAW velocity is slower in a ZnO substrate than in a GaAs substrate. The $S_{12}$ peak increases to $-60$ dB with the IDTs at the GaAs and ZnO interface (Fig. 4.7(b)), and $-55$ dB with the IDTs on the ZnO surface (Fig. 4.7(a)). Both values of $S_{12}$ with the ZnO layer show a clear resonance matching a $\text{sinc}$ function. The device with IDTs on the surface of the ZnO shows better SAW generation and propagation than that with IDTs at the ZnO/GaAs interface. This may imply that the piezoelectric coupling coefficient on the surface of the ZnO layer is better than at the GaAs/ZnO interface.

Alternatively, this difference may result from a difference in SAW detection efficiency in these two cases. On the ZnO surface, SAWs are generated from one IDT and well detected by the other IDT. At the interface, a set of IDTs generates SAWs. During propagation, SAWs will leak to the ZnO surface and reduce the detection efficiency of the other IDT, which is also at the GaAs/ZnO interface. This leakage may also explain the lower $S_{12}$ peaks at the interface than on the surface. This measurement shows that it is possible to deposit the IDTs at the GaAs/ZnO interface to improve the SAW amplitude. When the sample is dipped into liquid helium, we observe the $S_{12}$ peak decreases from $-60$ dB to $-80$ dB because of the mass-loading effect. However, the SAW resonance is not completely attenuated by the mass-loading, which also shows an improvement in SAW amplitude compared with the plain GaAs substrate. To maximise the SAW amplitude in the 2DEG, we
Section 4.3. Results and discussions

prefer to deposit IDTs at the GaAs/ZnO interface instead of on the surface.

Later IDTs of 1 µm SAWs are patterned using electron-beam lithography with finger width and separation of 250 nm. Fig. 4.9 shows the S-parameters in the SAW device on a GaAs heterostructure with and without a ZnO layer. In a GaAs heterostructure, the dip in the $S_{11}$ spectrum is around 2 dB at around 2.73 GHz, and the peak in the $S_{12}$ spectrum is around $-60$ dB with a background around $-100$ dB. This background signal is the direct coupling of electromagnetic radiation between two separate sets of IDTs. The higher the frequency, the stronger the background signal. With a ZnO layer, the dip in the $S_{11}$ spectrum increases to 10 dB and the position is shifted to 2.65 GHz. In a GaAs substrate, $S_{11}$ dip at $-6$ dB with a background of $-4$ dB gives the effective power-transfer efficiency is around 15 %. With ZnO, $S_{11}$ dip at $-15$ dB with a background of $-5$ dB the power-transfer efficiency increases to 30 %. In the $S_{12}$, the peak increase from $-60$ dB to $-50$ dB by depositing a ZnO layer. The bandwidth of $S_{12}$ is also greater than without a ZnO layer, as seen in Fig. 4.9(b). These results show a great improvement in SAWs with a ZnO layer on a GaAs substrate.

ZnO and GaAs have different SAW velocities and can build a slow-on-fast structure for SAW propagation. This ZnO overlayer allows other wave modes. Apart from the fundamental Rayleigh mode, we also observe a Sezawa mode at 3.3 GHz, as shown in Fig. 4.10. The Sezawa mode is weaker than the Rayleigh mode with the $S_{12}$ peak reaching only $-80$ dB. Once the chip is dipped into liquid helium, the Rayleigh mode is attenuated due to the mass-loading effect, but the Sezawa mode is not naturally attenuated inside the liquid helium (Fig. 4.10 (b)). At room temperature, ZnO is not perfectly insulating. High-density surface charges screen SAWs and strongly damp SAW propagation, as shown by blue lines in Fig. 4.10.

4.3.2 Enhancement in SAW-pumping

From $S$-parameter measurements, we have shown that the SAW amplitude is significantly increased with a ZnO overlayer, which demonstrates results similar to those of previous research. However, the improvement in SAW-pumping at the 2DEG,
Chapter 4. SAW enhancement in a ZnO/GaAs heterostructure

Figure 4.9: $S$-parameters $S_{11}$ (a) and $S_{12}$ (b) of 1 $\mu$m SAWs on a GaAs substrate with and without a ZnO overlayer.

Figure 4.10: Rayleigh (a) and Sezawa (b) modes of 1 $\mu$m SAW above (black lines), in (red lines) liquid helium and at room temperature (blue lines).

which is 90 nm below the surface, has not been investigated before.

Pedrós et al. have calculated the effective piezoelectric efficiency $K^2_{\text{eff}}$ as a function of the wavelength and thickness of the ZnO overlayer $kH$. In this device, we design the wavelength to be 1 $\mu$m with a ZnO overlayer thickness of 800 nm. From the calculation, the effective piezoelectric coupling coefficient is 0.4%, which is much higher than that of GaAs (0.06%). Meanwhile, we find that not only Rayleigh mode but also the Sezawa mode can pump electrons in the 2DEG.

To measure the SAW amplitude at the 2DEG, we utilise the classic SAW-pumping theory: the SAW pumped current is determined by the maximum gradient of the SAW potential waves and SAW channels. If the maximum slope of a SAW is higher than that of a SAW channel created by split gates, the electrons in 2DEG are trapped in the SAW minima and dragged across the SAW channel. As the maximum slope of the SAW channel increases, the SAW-pumping current decreases.
Figure 4.11: Pinch-off characteristics of a 1D channel with (black line) and without (red line) SAWs. The shift of pinch-off voltage is labelled $\Delta V_p$.

and is finally pinched off.

Figure 4.12: (a) Calculated required SAW amplitude, $A_{SAW}$, for the SAW channel as a function of pinch-off voltage, $V_p$, in the device without (red line) and with ZnO (black line). (b) Calculated and measured pinch-off voltages at different SAW powers in the device without (red line) and with ZnO (black line).

Beyond the 1D channel pinch-off, a potential barrier is raised above the Fermi level. In a standard HEMT wafer, the 2DEG is 90 nm below the surface, and the pinch-off voltage, $V_p$, is around $-1\,\text{V}$ for split gates length of $L = 1.5\,\mu\text{m}$ and width of $W = 0.7\,\mu\text{m}$. When SAWs are launched, $V_p$ is further shifted because of the existence of SAW-pumping. Experimentally, from the delay of $V_p$, we can estimate the SAW amplitude: the more negative $V_p$, the greater the SAW amplitude it is. In a pure GaAs heterostructure with a SAW at a power of 11 dBm, the delay of $V_p$ is around the 100-200 meV. With a ZnO layer, $V_p$ is significantly delayed up
to 630 meV by a SAW at the same power, as seen in Figure 4.11. This significant delay in \( V_P \) experimentally proves the enhanced amplitude of the Rayleigh-mode SAW with a ZnO overlayer on a GaAs heterostructure. It is noticeable that even without SAW-pumping \( V_P \) has already been shifted 0.2 V with a ZnO layer on the top, which is explained by the dielectric constant difference between ZnO and air at the interface (more details in Chapter 2).

![Figure 4.13: Calculated required SAW power as a function of \( V_{SG} \). In Model 1, a smooth SAW channel is used in the simulation (black line). In Model 2, random impurities (Gaussian potentials with an amplitude of 10 meV and width of 100 nm) are introduced into the entrance of the SAW channel (red line). Inset: SAW potential at \( V_{SG} \) from -0.6 V to -1.4 V with random impurities. The red asterisks show the position of the maximum gradient in the SAW channel.](image)

According to the classic SAW-pumping theory, for a given \( V_P \), if we know the maximum slope of the SAW channel, we can deduce the maximum gradient of the SAW. Assuming the SAW is a sine wave, we can calculate the amplitude of the SAW. The potential profile of a SAW channel is calculated by solving the electrostatic Poisson equation at different values of \( V_{SG} \) using Nextnano (more details in Chapter 2). Fig. 4.12(a) demonstrates the calculated required SAW amplitude as a function of \( V_{SG} \) for SAW devices with and without a ZnO overlayer. After that the SAW amplitude measured in meV is converted to SAW power in a unit of dBm, and this matches the experimental results very well, as seen in Fig. 4.12(b). From the model, we find that SAW amplitude improves to 100 meV at a power of 11 dBm with the help of a ZnO layer, which is much higher than that on the GaAs substrate at the same power (around 25 meV). In the ZnO-coated SAW device, the modelled \( V_P \) at different RF powers does not exactly match experimental results. There are small deviations at \( V_P = -0.7 \) V and -1 V. In this model, the entrance of the SAW channel has a smooth potential. In real devices, there are impurities randomly distributed in the SAW channel. We introduce impurities by adding the Gaussian potential with a small amplitude at the entrance of the SAW channel, as shown in the inset of Fig. 4.13. By comparing the maximum gradient of the channel and the SAW, we can recalculate the required SAW amplitude as a function of \( V_{SG} \).
The model indicates clear deviations matching the experimental results, as seen in Fig. 4.13.

### 4.3.3 Sezawa-mode wave pumping

In scattering measurements, as well as the Rayleigh mode, we also observe the Sezawa mode. Here we discuss the Sezawa-mode pumping in a ZnO/GaAs heterostructure. A Sezawa wave is a plate wave with an asymmetric mode. In other words, the Sezawa mode is more confined in the ZnO layer, and the effect on the 2DEG should be smaller than the Rayleigh mode. At a voltage beyond the 1D channel pinch-off, we sweep the frequency from 2.5 GHz to 3.5 GHz. There are two central peaks at around 2.6 GHz and 3.3 GHz, as shown in Fig. 4.14. The strong peak at 2.6 GHz results from the fundamental Rayleigh mode, and the weak peak at 3.3 GHz results from the first Sezawa mode. However, $V_{SG}$ need to be set less negative to observe the Sezawa mode pumping. These results prove that the Sezawa mode can also penetrate into the 2DEG and pump electrons, but the efficiency is much lower than it with the fundamental Rayleigh mode.

In the SAW-pumping experiments in a GaAs/AlGaAs heterostructure, we observe the quantised acoustoelectric current, $I = N_e f$, using the Rayleigh mode. For the Sezawa mode, we fail to realise a quantised current. Theoretically, to see quantised acoustoelectric current, strong transverse and longitudinal confinement are both essential for creating dynamic quantum dots. The amplitude of the Sezawa mode at 90 nm below the interface is weak. Therefore the longitudinal confinement of the DQDs is not sufficient to achieve quantised acoustoelectric current with a fixed number of electrons in SAW minima.

### 4.3.4 Enhancement in SAW quantisation

The SAW-driven quantised current is one of the most well-known features in SAW electron pumping. On a GaAs substrate, the SAW resonant frequency is around

![Figure 4.14: Pumping current with the Rayleigh mode waves (a) ($V_{SG} = -0.85$ V) and first Sezawa mode waves (b) ($V_{SG} = -0.75$ V).](image-url)
2.75 GHz, the first SAW-driven plateau is at about 0.44 nA and the second plateau is at 0.88 nA. From previous measurements, if the SAW power is too weak, the SAW amplitude is not strong enough to define dynamic quantum dots, and hence there are no SAW-driven quantised plateaus. As the RF power increases, the SAW amplitude increases and becomes strong enough to provide strong longitudinal confinement and form the quantised plateaus. Usually, an RF power of 3 dBm is needed to observe SAW-pumping current and 9 dBm is needed for the quantised current, as shown in Fig. 4.15(a). This required RF power varies from device to device, and unpredictable wafer defects and the lithographic errors can affect the SAW efficiency.

Figure 4.15(b) shows the quantised SAW current in a SAW-device with a ZnO layer at an RF power from $-5$ dBm to $-2$ dBm, and Fig. 4.16 shows same measurements from $-6$ dBm to 11 dBm in an increment of 0.2 dBm. At an RF power of $-4$ dBm, the SAW-pumping negative current appears. As the RF power increases to $-3$ dBm, SAW quantisation begins to show up with a few plateaus. However, as the RF power increases, the SAW quantisation begins to be lost and even disappears. More interestingly, as RF power continually increases, SAW quantisation appears again. Figure 4.16 shows the evolution of SAW-driven current plateaus at different SAW powers. These SAW plateaus disappear and reappear twice in the RF power region from $-6$ dBm to 11 dBm. We explain this phenomenon as being a consequence of randomly-distributed impurities in the SAW channel. These impurities
modulate the entrance of the SAW channel and then modulate the dynamic quantum dots. Therefore the impurities play an important role in SAW quantisation. As \( V_{SG} \) becomes more negative, the SAW channel can overcome impurities, and SAW quantisation recovers.

<table>
<thead>
<tr>
<th>RF power</th>
<th>GaAs</th>
<th>ZnO/GaAs</th>
</tr>
</thead>
<tbody>
<tr>
<td>Acoustoelectric current</td>
<td>3 dBm</td>
<td>−5 dBm</td>
</tr>
<tr>
<td>Quantised current</td>
<td>9 dBm</td>
<td>−3 dBm</td>
</tr>
</tbody>
</table>

Table 4.2: Required SAW powers in SAW devices.

Figure 4.16: SAW-driven current as a function of \( V_{SG} \) at different RF powers from −6 dBm to 11 dBm in increments of 0.2 dBm.

From the results of the experiments, the ZnO overlayer can significantly reduce the required RF power so that the SAW-pumping effect and quantised plateaus can be observed in a GaAs heterostructure, as shown in Table 4.2. The minimum RF power required to observe SAW acoustoelectric current is reduced to around −5 dBm and the minimum RF power required to observe SAW quantised plateaus decreases to around −3 dBm. A reduction in RF power indicates an improvement in SAW amplitude at 2DEG with a ZnO layer on a GaAs substrate. In low-temperature measurements, the high RF power causes serious heating and increases the electron temperature. With the help of ZnO, we can reduce RF power to avoid unnecessary heat dissipation in measurements.

From these measurements, it can be seen that the SAW amplitude improves with the ZnO layer. However, the enhancement in the accuracy of SAW quantisation is not evident. The improved SAW amplitude increases the longitudinal confinement of the SAW dynamic quantum dot. Fig. 4.17 compares the calculated transverse confinement for the same \( V_{SG} \) on the SAW device with and without a ZnO overlayer. Due to the different dielectric layers, the simulation shows that transverse confinement is weaker in a device with a ZnO layer than with one without a ZnO layer. Moreover, non-adiabatic errors may still be an important limitation to the accuracy of SAW quantisation, even with the help of ZnO.
Figure 4.17: Calculated electrostatic transverse confinement for $V_{SG} = -1.1\,\text{V}$ in GaAs heterostructures with and without a ZnO overlayer. The potential is fitted to a parabolic function.

4.3.5 SAW-pumping in liquid helium

Figure 4.18: SAW-quantised current oscillation in liquid helium at different powers (a) 0 dBm, (b) 2 dBm, (c) 3 dBm, (d) 5 dBm, (e) 9 dBm, (f) 11 dBm. The red line shows the SAW quantised current above the liquid helium.

As mentioned before, both Rayleigh mode and Sezawa mode can still propagate immersed in liquid helium, although the Rayleigh mode is strongly attenuated because of mass-loading. Without a ZnO layer, the Rayleigh mode is strongly damped by liquid helium, and the SAW-pumping current disappears. One problem in SAW measurements in a He dewar is the unstable temperature. To avoid mass-loading, we usually place the sample holder above the liquid. During measurements, the helium boils off, and the liquid level drops and the temperature above it of the sample increases. If the measurement can be performed immersed in liquid helium, the temperature is stable at 4.2 K during the measurements. We have shown that
a ZnO overlayer can improve the SAW amplitude. Therefore it is still possible to perform SAW-pumping in liquid He.

Figure 4.18 shows the SAW-pumping current inside the liquid helium with a ZnO overlayer. We find strong oscillations in the acoustoelectric current. The red curve in Fig. 4.18 shows the SAW-pumping current when the device is right above the liquid helium. The black curve in Fig. 4.18 demonstrates the SAW-pumping current when the device is dipped into the liquid helium. Inside the liquid helium, the SAW-pumping current oscillates between zero and the red line. The peak of oscillation matches the SAW-pumping current above the liquid helium (red line). The first SAW quantised plateau clearly shows, even the sample is inside liquid helium. More interestingly, the period of oscillations decreases as the SAW power increases. The RF power starts from $-6 \text{ dBm}$, when the oscillation period is about $10 \text{ s}$. As the power increases, the oscillation period becomes shorter and shorter. When the power reaches $11 \text{ dBm}$, the oscillation disappears, and the SAW-pumping currents outside and inside the helium overlap, which demonstrates that the mass-loading has been overcome and the same SAW amplitude is maintained in the liquid.

![Figure 4.19: SAW-pumping current oscillation period as a function of RF input power in units of mW. The model shows an inverse proportional relationship ($y = 26.5/(x + 1.6)$) between the period and the power. Inset: period as a function of RF power in units of dBm.](image)

We explain this SAW-pumping current oscillation using a gas buffer layer. Because of the good piezoelectric coupling in ZnO, the power transfer in IDTs is more effective than in GaAs, which is shown in $S_{11}$ measurements. When an RF signal is applied to the transducers, the SAW oscillation transfers some of its energy and momentum to the liquid, causing heating, and hence gas bubbles or a gas buffer layer. This helium gas layer reduces the mass-loading and energy transfer. However, the liquid helium quickly cools down and re-condensed the gas buffer layer. When the buffer layer disappears, the mass loading recovers and the SAW-pumping current drops to zero and the process repeats. When the RF power is high enough, it continuously creates a helium gas buffer layer. As shown in Fig. 4.18(f), at $11 \text{ dBm}$ of...
RF power, the helium gas can separate the liquid helium and ZnO interface continuously, preventing the mass loading. The RF-power-dependent oscillation period is given in Fig. 4.19. There is an inverse proportional relationship between the period of oscillation and the SAW power, here is SAW power need to be calibrated from the RF power. From the production of the two variables, the energy required to reach thermal equilibrium is a constant of 27 mJ.

### 4.4 Conclusion

In this chapter, we have grown the high-quality ZnO on an AlGaAs/GaAs heterostructure using HiTUS and reported a strong enhancement in SAW amplitude. To protect the 2DEG during sputtering, we deposit a thin Al$_2$O$_3$ buffer layer using ALD. With the help of the ZnO layer, the efficiency of RF power conversion to the SAW power is greatly improved to 30%. In SAW-pumping measurements, we observe quantised SAW current at a much lower power for a given gate voltage than without a ZnO overlayer. From the pinch-off voltage, we estimate that the SAW amplitude improves to 100 meV at an RF power of 11 dBm. Just as for the Rayleigh mode, the Sezawa mode can also pump electrons in the 2DEG, but the current is not quantised. When we dip the device into the liquid helium, the SAW-pumping current oscillates with a fixed period, which can be explained by a heat-induced gas buffer layer. All these measurements show the successful growth of a ZnO thin film on a GaAs heterostructure. However, the accuracy of SAW quantised plateaus is not significantly improved. This observation indicates that the weak SAW amplitude may not be the main limitation of SAW quantised pumping, and other error mechanisms need to be considered, such as non-adiabatic errors.
Quantised conductance of 1D strongly-correlated electrons in a ZnO heterostructure

In Chapter 4, we have discussed the fabrication and measurement of SAW devices in a ZnO/GaAs heterostructure, and find it is not straightforward to grow high-quality ZnO on a GaAs heterostructure without damaging the 2DEG. In physics, it will be beneficial to combine the high-quality 2DEG with a ZnO heterostructure. In 2007, Tsukazaki et al. developed a MgZnO/ZnO heterostructure and created a high-quality 2DEG at the heterointerface. This ZnO heterostructure makes it possible to have a high-quality 2DEG and strong piezoelectric coupling. However, the development of this ZnO heterostructure is still at an early stage.

Here we report ballistic transport in a high-quality MgZnO/ZnO heterostructure and show clear 1D conductance quantisation. Using DC-bias spectroscopy and in-plane magnetic-field measurements, we find the g-factor in a ZnO 1D wire is enhanced by a factor of $\sim 3$ compared to the bulk and is relatively constant at low 1D subband indices. Additionally, we show that the electron effective mass increases as the density decreases in our 1D systems, as occurs for 2D electron systems with similar heterostructures. Furthermore, we also observed apparent 'N.7' structures in 1D subbands with a higher 1D subband index $N$, which behave in a manner consistent with the 0.7 structure in a GaAs quantum wire.

This work involves a collaboration with Dr Yusuke Kozuka and Professor Masashi Kawasaki from the University of Tokyo, who provided the MgZnO/ZnO wafers for our experiments.

5.1 Introduction

Physical phenomena in transition-metal oxides and their complex compounds have stimulated intense interest in research, covering metallic, semiconducting, and insulating properties. At the heterointerface of two oxide layers, a symmetry-breaking leads to novel properties including quantum confinement of electrons, superconductivity, and ferromagnetism. Because of these fascinating features, the oxide heterostructure is becoming more and more popular in condensed-matter physics. However, the growth technique for oxide heterostructures is tricky, especially the control of oxygen vacancies, which affects the physical properties of the oxide het-
Figure 5.1: (a) Temperature-dependent mobility, $\mu$, of 2DEG in ZnO heterostructures grown by different techniques. (b) Quantum Hall measurement of a high-quality MgZnO/ZnO heterostructure with $\mu > 1 \times 10^6$ cm$^2$/Vs. Figures from Ref. 119.

5.1.1 2DEG in a MgZnO/ZnO heterostructure

In an AlGaAs/GaAs heterostructure, modulation-doping in the AlGaAs layer creates large electric fields. In a MgZnO/ZnO heterostructure, the lattice constants of Mg$_x$Zn$_{1-x}$O and ZnO are different, where $x$ is the Mg content. This lattice mismatch creates a strong strain at the interface between them. Because ZnO is a piezoelectric material, the large strain rises a large built-in electric field. ZnO is a wurtzite crystal, which has spontaneous charge polarisation. The mismatch in the spontaneous and piezoelectric polarisation in the MgZnO and ZnO layers creates a 2DEG at the interface. This mechanism is different from what happens in an AlGaAs/GaAs heterostructure, but similar to that in an AlGaN/GaN heterostructure.

Early in 2007, Tsukazaki et al. grew a MgZnO/ZnO heterostructure using pulsed atomic layer deposition (PLD) and observed the quantum Hall effect and Shubnikov–de-Haas (SdH) oscillations. Due to the limitations of the growth technique, the electron mobility never exceeded $1 \times 10^4$ cm$^2$/Vs. MBE was then used instead of PLD, and the electron mobility reached $1 \times 10^5$ cm$^2$/Vs. The even-denominator fractional quantum Hall effect demonstrates unique properties of this ZnO heterostructure. Most recently, the MBE technique has been modified with an ozone condition, and the 2DEG density can reach $1 \times 10^{11}$ cm$^{-2}$ with electron mobility of more than $1 \times 10^6$ cm$^2$V$^{-1}$s$^{-1}$, as shown in Fig. 5.1. These 2D transport measurements show that the electric properties of the 2DEG in a ZnO heterostructure can compete with that in conventional III-V heterostructures.

Here we briefly introduce the growth of a MgZnO/ZnO heterostructure using by MBE. The substrate is a Zn-polar single-crystal substrate grown by hydrothermal methods, and the surface is polished to be atomically flat. After pre-etching using an HCl solvent (HCl:H$_2$O=7:200), the substrate is mounted on a pure quartz holder, which can reduce the contamination from the sample holder. At a high temperature of around 920 °C, the ZnO or MgZnO thin film is grown by radical oxygen sources.
Section 5.1. Introduction

with high-purity fluxes of Zn (7N purity) and Mg (6N purity). In the growth, the II/V flux ratio is controlled, which can tune from an O-rich condition to a Zn-rich condition during the growth.

In a similar way to varying Al content in an AlGaAs/GaAs heterostructure, we can engineer the band structure of the Mg$_x$Zn$_{1-x}$O by controlling Mg content, $x$, creating a band discontinuity at the interface. With the help of the built-in solver in Nextnano, we calculate the strain and piezoelectric electric fields. Figure 5.2(a) shows the conduction band in a MgZnO/ZnO heterostructure. It clearly shows that the edge of the conduction band at the heterointerface is below the Fermi level. The inset in Fig. 5.2(a) shows the electron density at the heterointerface. Fig. 5.2(b) and (c) demonstrates the 2DEG density, $n_{2D}$, as a function of Mg content, $x$, and the thickness of the MgZnO layer. As $x$ increases, $n_{2D}$ increases linearly, from $1 \times 10^{11}$ cm$^{-2}$ at $x = 0.01$ to $5 \times 10^{12}$ cm$^{-2}$ at $x = 0.1$. As the MgZnO thickness increases with a fixed $x = 0.02$, $n_{2D}$ increases significantly and saturates at around $8 \times 10^{11}$ cm$^{-2}$ at a MgZnO thickness of 500 nm.

Figure 5.2: (a) Conduction band of a MgZnO/ZnO heterostructure simulated by Nextnano. (At the interface the wave function of the ground state and the first excited state are plotted as red and blue lines.) Inset: Distribution of electron density along the $z$-axis. The 2DEG density, $n_{2D}$, as a function of Mg content, $x$, (b) and thickness of the MgZnO layer (c).
5.1.2 Strongly-correlated electrons in a ZnO heterostructure

The strength of electron-electron interaction is quantified by the ratio of Coulomb energy, $E_C$, to kinetic energy, $E_K$, which is called the Wigner-Seitz parameter, $r_S$:

$$E_C = \frac{e^2}{4\pi \varepsilon (\pi n_{2D})^{-1/2}}$$  \hspace{1cm} (5.1)

$$E_K = \frac{\hbar^2 k_F^2}{2m^*}$$  \hspace{1cm} (5.2)

$$r_S = \frac{E_C}{E_K} = \left(\frac{\pi n_{2D}}{m^* e^2}\right)^{-1/2} \frac{\pi n_{2D}}{4\pi \varepsilon \hbar^2}$$  \hspace{1cm} (5.3)

where $\varepsilon$ is the dielectric constant, the Fermi wavenumber $k_F = \sqrt{2\pi n_{2D}}$, and $n_{2D}$ is 2DEG density. According to Eqn. 5.3, the high electron effective mass ($0.3 m_e$ for bulk ZnO) and the low dielectric constant ($8.3$) result in a stronger electron-electron interaction even than for the holes in GaAs (with a similar $m^*$ but a larger $\varepsilon$).

Figure 5.3 (a) compares the transport-scattering time, $\tau_{tr}$, as a function of $r_S$ in different materials. When $r_S$ reaches 10, the electron scattering time is significantly degraded in a GaAs heterostructure owing to disorders. However for ZnO, $\tau_{tr}$ is two orders of magnitude higher than it in GaAs.$^{120}$

![Figure 5.3](image.png)

Figure 5.3: (a) Comparison of $\tau_{tr}$ as a function of $r_S$ in GaAs,$^{121,122}$ GaN,$^{123}$ Si/SiGe,$^{124}$ and ZnO. Figure from Ref. 120. (b) Measured $m^*_{CR}$ and $m^*_{tr}$ in MgZnO/ZnO heterostructures with different 2DEG densities, from $1.3 \times 10^{12}$ cm$^{-2}$ to $2 \times 10^{11}$ cm$^{-2}$. Figure from Ref. 125.

The strength of electron correlation can also be expressed by electron effective mass, $m^*$. Kasahara et al. compared $m^*$ measured by cyclotron resonance and Shubnikov–de-Haas oscillation. In cyclotron-resonance measurements, radiation only couples to the centre of mass of the electron motion, not including the interaction with neighbouring electrons. This effective mass is labelled $m^*_{CR}$. In electron
transport measurements, electron-electron interaction is considered because of the quasi-particle dragging effect. This effective mass is labelled $m^*_{tr}$. Figure 5.3(b) compares $m^*_{CR}$ and $m^*_{tr}$ in MgZnO/ZnO heterostructures with different 2DEG densities. It clearly shows that $m^*_{CR}$ is constant around 0.3 $m_e$. In contrast, $m^*_{tr}$ increases as the density decreases. This is because that the electron-electron interaction energy becomes greater as the density decreases. A similar effect is observed in other 2DEG systems, such as AlGaAs/GaAs,$^{126}$ AlGaAs/AlAs,$^{127}$ and Si-based MOSFET.$^{128}$ From a Green’s function Monte Carlo calculation, Wigner crystallisation is predicted at $r_S \sim 37 \pm 5$, where can realise the spontaneous ferromagnetic transition.$^{129}$ This Wigner crystallisation has not been verified in 2DEGs at zero magnetic field, and the 2DEG in a MgZnO/ZnO heterostructure provides a promising candidate for investigation of Wigner crystallisation.

5.1.3 Spintronics in a ZnO heterostructure

Because of the net nuclear spin in most Ga and As isotopes, the conventional GaAs heterostructure is not a good candidate for spintronics. Only 4% of Zn atoms are $^{67}$Zn with 5/2 nuclear spin, and other Zn isotopes have even number of neutrons and so no net nuclear spin. The ZnO heterostructure also shows weak spin-orbit interaction. The Rashba parameter is $7 \times 10^{-14}$ eVm, which is the second smallest value among semiconductor heterostructures, only larger than Si/SiGe.$^{130}$ In electron spin resonance measurement, the spin relaxation time $T_2^*$ is estimated at a maximum value of 27 ns.$^{130}$ The spin susceptibility $g^*m^*$, where $g^*$ is the Landé $g$-factor, is important in spintronics. In a MgZnO/ZnO heterostructure, $g^*$ is measured at around 2, and $m^*$ is 0.3 $m_e$. Both of these are larger than the equivalent values in GaAs ($g^*=-0.44$, $m^* = 0.067 m_e$). All of these show that the ZnO heterostructure provides a promising candidate for quantum spintronics.

5.1.4 Mesoscopic physics in oxide heterostructures

Except for controlling the Mg content in Mg$_x$Zn$_{1-x}$O during the MBE growth, we can tune the 2DEG density with external electric fields using surface gates. Well-established semiconductor technologies are dominated by gate-controlled devices such as a metal-oxide-semiconductor field-effect-transistor (MOSFET) and a high-electron-mobility-transistor (HEMT). Many low-dimensional nanostructures are created using lithography and metallic gates, such as 1D quantum wires or 0D quantum dots. However, gating oxide heterostructures is challenging. The 2DEG density in a MgZnO/ZnO heterostructure was tuned by gating on a thin layer of amorphous Al$_2$O$_3$. However, this Al$_2$O$_3$ insulator may trap electrons at the surface of the insulator layer. We found that the Al$_2$O$_3$ insulator damages or adds the 2DEG in a high-quality ZnO heterostructure (more details will be discussed later). To avoid the insulator, a conducting polymer poly(3,4-ethylendioxythiophene):poly(styrenesulfonate) (PEDOT: PSS) creates a stable Schottky junction and provide external electric fields to tune the 2DEG density in the MgZnO/ZnO heterostructure.$^{131}$ Alternative techniques can also create nanostructures in oxide heterostructures, such as conducting atomic force microscope (C-AFM) lithography on a LaAlO$_3$/SrTiO$_3$ heterostructure, which shows quantised conductance in units of $e^2/h$ in a strong magnetic field.$^{132-134}$
Chapter 5. Quantised conductance of 1D strongly-correlated electrons in a ZnO heterostructure

We use quantum point contacts (QPCs) to create quantum wires in a MgZnO/ZnO heterostructure. In a quantum wire, the lateral electrostatic confinement creates a series of 1D subbands, through which electrons travel between 2D leads and two Ohmic contacts. If a small bias $V$ is applied to the left contact, so that the chemical potential $\mu_L = \mu - eV$, and the right contact is at the chemical potential $\mu_R = \mu$. Provided that there is no scattering into a backward-going subband, the current passing to the left, $I_i^+$, or right, $I_i^-$, in small energy range $dE$ in the $i^{th}$ subband

$$dI_i^+ = -ev_i^E f(E, \mu - eV) \frac{1}{2} \frac{dn_i}{dE} dE, \quad (5.4)$$

where $v_i^E$ is group velocity at energy $E$ in subband $i$:

$$v_i^E = \frac{1}{\hbar} \frac{dE_{k_x,i}}{dk_x}, \quad (5.5)$$

and $f(E, \mu - eV)$ is the Fermi-Dirac distribution function

$$f(E, \mu) = \frac{1}{1 + e^{(E-(\mu-eV))/k_B T}}. \quad (5.6)$$

From 1D density of states $\frac{dn_i}{dE} = \frac{2}{\pi} \frac{dk_x}{dE}$, Eqn. 5.4 becomes

$$dI_i^+ = -\frac{2e}{h} f(E, \mu - eV) dE, \quad (5.7)$$

and similarly

$$dI_i^- = -\frac{2e}{h} f(E, \mu) dE. \quad (5.8)$$

Figure 5.4: Quantised conductance in units of $2e^2/h$ in GaAs wires. Figure from Ref. 9.
Section 5.2. Device fabrication

The total current between two Ohmic contacts through the $i^{th}$ subband is derived by

$$I_i = \int (dI_i^+ - dI_i^-) = \frac{2e}{h} \int_{-\infty}^{\infty} (f(E, \mu) - f(E, \mu - eV))dE \quad (5.9)$$

Therefore the final current over $N$ subbands is

$$I = \sum I_i = N \frac{2e^2}{h} V \quad (5.10)$$

Conductance is expressed as $G = I/V = N \times 2e^2/h$, where $N = 1, 2, 3, \cdots$. The quantisation of conductance in integer multiples of $2e^2/h$ is a signature of ballistic charge transport in 1D systems. The lateral electrostatic confinement creates a series of 1D subbands, in which spin-up ($\uparrow$) and spin-down ($\downarrow$) subbands each contribute $e^2/h$. This is already observed in many materials, including GaAs/AlGaAs (seen in Fig. 5.4), InGaAs/InAlAs heterostructures, strained epitaxial germanium, and carbon-based materials.

5.2 Device fabrication

In nanotechnology, we can create a quantum wire using lithography and etching. However, the etching process is difficult to control accurately. Once a quantum wire is etched, the confinement is difficult to vary. Alternatively, the field-effect transistor is more popular than etching. When negative voltages are applied to QPCs, free electrons below gates are depleted, defining a quasi-1D wire. By sweeping voltages, we can modulate the transverse confinement. Thus the QPC technique is flexible and controllable in the investigation of 1D physics. Here in a MgZnO/ZnO heterostructure, we optimise the fabrication process and succeed in creating ballistic quantum wires using QPCs in a MgZnO/ZnO heterostructure.

5.2.1 Wafers

There are two batches of wafers used in this work, as shown in Table 5.1. The first batch contains ZnO heterostructures with a thick MgZnO layer (500 nm). The second batch contains ZnO heterostructures with a thin MgZnO layer (around 100 nm, grown especially at our request). In each batch, there are two wafers with different densities and mobilities (one high $n_{2D}$ with low $\mu$, and one low $n_{2D}$ with high $\mu$). The ZnO substrate is roughly transparent with snow-flake features in the substrate, as seen in Fig. 5.5. Because of the transparency, we have to be careful in fabrication and to distinguish the polished top surface.

Figure 5.5: Snow-flake features in a single-crystal ZnO substrate.
The ZnO wafer is only 5 mm × 5 mm in size, which is much smaller than a GaAs wafer. We cleave the chip into two pieces each with dimensions of 5 mm × 2.5 mm, and each piece contains two devices with dimensions of 2 mm × 2 mm. The single-crystal ZnO substrate is very difficult to cleave. With a GaAs substrate, we only use the diamond scriber to scribe once or twice and then can cleave it easily. However, for a ZnO substrate, several dozen scribes are required before the chip can be cleaved. After scribing, we usually use a toothpick to press the corner of the GaAs wafer to break the chip following the scribing lines. However, there is a risk of breaking the ZnO substrate into random pieces. Therefore this dangerous operation should be avoided. Instead we use the scriber to cleave the ZnO substrate until it breaks without extra pressing. The device fabrication process is similar to that for a SAW-device in a GaAs heterostructure with mesa, Ohmic contacts, and surface gates, as shown in Fig. 5.9(a)-(d).

<table>
<thead>
<tr>
<th>Wafer</th>
<th>$h_{\text{MgZnO}}$ (nm)</th>
<th>Density $n_{2\text{D}}$ (cm$^{-2}$)</th>
<th>Mobility $\mu$ cm$^2$/Vs</th>
</tr>
</thead>
<tbody>
<tr>
<td>Zn5-1</td>
<td>500</td>
<td>$1.1 \times 10^{12}$</td>
<td>$8.3 \times 10^4$</td>
</tr>
<tr>
<td>Zn5-2</td>
<td>500</td>
<td>$3.1 \times 10^{11}$</td>
<td>$5.2 \times 10^5$</td>
</tr>
<tr>
<td>Zn1-1</td>
<td>92</td>
<td>$3.7 \times 10^{11}$</td>
<td>$3.8 \times 10^5$</td>
</tr>
<tr>
<td>Zn1-2</td>
<td>97</td>
<td>$7.8 \times 10^{11}$</td>
<td>$7.8 \times 10^5$</td>
</tr>
</tbody>
</table>

Table 5.1: Wafer assessments at $T = 0.5$ K in dark.

5.2.2 Mesa etching

Once the wafer is cleaved and cleaned with acetone and IPA, a Hall-bar mesa is patterned using optical lithography. The piece of wafer is small, only 2.5 mm × 5 mm, and there is a narrow gap between the device and the edge of the chip. The photoresist edge-bead effect is problematic. First, we increase the spinning speed from 5500 rpm to 6500 rpm, and perform an edge-bead removal step. After the pattern is developed, the chip is re-baked at 115 °C for 1 min to harden the photoresist. In a GaAs SAW device, the chip is usually dipped in HCl to remove the oxide. However, in the ZnO heterostructure, this process must be avoided because the HCl etches ZnO at a fast rate of 100 nm/s.

To etch ZnO controllably, we use an Ar-ion milling technique, which was performed by Dr. Jun-wei Liao or Dr. Rhodri Mansell. In the milling process, the beam current is controlled at 28 mA with 300 V acceleration. The etching rate depends on the incidence angle of the Ar-ion beam to the substrate. Figure 5.6 compares the etching profile of device milled at different angles. For the same milling process, the milling depth is about 590 nm at normal incidence, which is around half of that at 45°. The fast milling rate reduces the heating during the milling. However, mesa profile milling at 45° shows sharp peaks at the edges of the mesa, as shown by the black line in Fig. 5.6. Ion milling is the reverse process of sputtering deposition. These sharp peaks may come from the re-deposition of ZnO at the edge of the mesa, which may cause troubles in later fabrication and measurements. Therefore we choose to mill at 90° to avoid the ZnO re-sputtering. To prevent over-heating, we set a 100 s/50 s on-off ratio and wait half an hour after ten cycles. After several calibrations, the milling rate is around 14 nm/min. To ensure full removal of
the 2DEG, we set the milling target depth 50-100 nm past the depth of the 2DEG. Meanwhile, the Ar-ion beam also etches the photoresist at a similar rate, so the thickness of the photoresist has to be greater than the etching depth.

### 5.2.3 Ohmic contacts

For ideal Ohmic contacts, we need the Schottky barrier height to be zero. Figure 5.7 demonstrates the Schottky barrier height of different metals on ZnO. Ti, Al, In, and Ta can be used as Ohmic metals for ZnO. In our devices, we compare the Ti/Au and Al and find that the Al contacts are difficult to bond, which may be because of the natural oxide layer on Al. Therefore, we choose the Ti as an Ohmic metal and a thick Au layer for bonding. After the Hall-bar mesa, Ohmic contacts are patterned and metallised with Ti/Au (20 nm/100 nm), and thermal annealing is not necessary. To make sure of good contact between the Ti/Au layer and a deep
mesa, we use a rotating stage at an angle of incidence of 45° in the evaporator. At a low temperature of 4 K, we measure the contact resistance, which is around 1 kΩ.

5.2.4 Quantum point contacts

The Schottky junction is one of the most fundamental parts of a field-effect transistor. The large ionicity creates the Schottky limit in an oxide heterostructure. In ZnO, the Schottky barrier strongly depends on surface conditions, polarisation and other conditions. It is difficult to create a strong and reliable Schottky barrier for ZnO with a metal such as Au, Pt unless special surface treatments are carried out. For example, the Au/ZnO Schottky junction strongly depends on the condition of the ZnO surface. The Schottky barrier height varies from 1.2 eV to 0 for different conditions of the ZnO, as shown in Fig. 5.7. Therefore it is difficult to apply Au directly to ZnO to form a field-effect transistor. Nakano et al. developed the deposition of PEDOT:PSS to create the Schottky junction for the ZnO, with Schottky barrier ranging from 0.7 to 1.2 eV. In metal-oxide field effect transistors, a thin layer of SiO₂ or Al₂O₃ is deposited at the surface to prevent current leakage through gates. We first deposited a 30 nm-thick Al₂O₃ insulator on a MgZnO/ZnO heterostructure using atomic-layer deposition (ALD). For the wafer with a high-density 2DEG (Zn5-1), the Al₂O₃ layer succeeds as a field-effect transistor, and no parallel conduction is observed. However, for a wafer with a low-density 2DEG (Zn5-2), we find strong parallel conduction in the sample. More details will be given in a later section. The reason for the extra conduction in the low-density wafer is not apparent. We lowered the temperature during the ALD process down to 120°C and saw no improvement. Hence the temperature should not be the reason for the damage. To overcome this problem, we developed another insulator material parylene-C, and the chemical structure of the parylene-C is shown in Fig. 5.8. With the help of Mr Dean Kos in Nano Photonic group, we deposited a thin-layer (30 nm) of parylene-C at room temperature, uniformly covering the mesa. After patterning on parylene-C, we etch the unwanted parylene-C insulator using plasma ashing for 3 mins at a rate of around 20 nm/min. Eventually, QPCs are patterned with electron-beam and optical lithography and metallised with Ti/Au. In the above process, there are a few important points that need to be considered:

- After patterning of the parylene-C insulator, any plasma ashing must be
avoided. Meanwhile, parylene-C consists of a soft polymer, and it can be easily damaged by scratches. Therefore, any hard contact must be avoided, such as tweezers scratches or ultrasonic vibrations.

- In the metal lift-off process, we soak the chip in SVC-14 solvent at room temperature for 1-2 days. Usually, we would heat the SVC-14 solvent to 70°C to speed up the lift-off process. However, we find that the heated SVC-14 solvent can dissolve the parylene-C, leaving a large number of pin-holes on the surface.

- We found that some of the ZnO substrates do not provide good insulation, even at low temperatures. The resistance between the gate and the Ohmic contacts can be hundreds of kΩ. This finite resistance causes trouble for low-conductance measurements. To avoid leakage, we extended the parylene-C
insulator under the bonding pads of the gate contacts, leaving no direct contact between the gate and the ZnO substrate.

5.2.5 Packaging

After fabrication, we attach a device to a LCC 20-pin package using GE vanish, as seen in Fig. 5.9(e). Ohmic contacts can be directly bonded with a ball bonder. However, there is a soft insulator under the bonding pads of gates. Therefore direct bonding with a bonder is impossible. In this case, we manually attach wires to the gates as follows. After making a bond the LCC package with the bonder, the Au bond wire is broken at a suitable length, with one end attached to the package and the other end suspended. This end of the wire is manually bent with sharp tweezers or a needle so that it comes into contact with the gate bonding pad on the device. We then use silver epoxy (silver paste and silver epoxy mixed in a 1:1 ratio) to stick this end of the wire to the bonding pad. In the bonder, the stage temperature is usually set at 120°C. We lower this temperature to 80°C to prevent the silver epoxy from spreading too much and shorting the other contacts. It is necessary to be careful during this step. The applied silver epoxy has to be small enough to cover only the bonding pad with a dimension of 100 µm × 100 µm. Figure 5.9(f) shows an example of such a bonded device, showing a sliver-epoxy shorting between two contacts (as the red text in Figure 5.9(f)). We then bake the chip at 180°C for 5 mins to harden the silver epoxy. After baking, if the silver epoxy spreads and shorts others contacts, we need to remove the epoxy residue with a sharp needle to clean the gap between the contacts.

5.3 Measurements

5.3.1 Characterisation of QPCs

Figure 5.10: Conductance and leakage current of two quantum wires with the same dimensions in device Zn5-1A as a function of $V_{SG}$. Inset in (a): conductance oscillations from Coulomb blockade at low conductance.
Section 5.3. Measurements

After the device is carefully bonded, we test the device at 4 K in a helium dewar. We apply a small bias (0.1 mV) oscillating at 77 Hz to the Ohmic contacts and measure the conductance with a lock-in amplifier. A SMU applies a negative voltage, $V_{SG}$, to the gates and also measures the leakage current through the gates. To protect the QPCs, we use RCR gate filters ($R = 1 \, \text{M} \, \Omega$ and $C = 0.1 \, \mu \, \text{F}$) to prevent a sudden change in gate voltage. In this device characterisation, we use a two-terminal measurement, and the measurement circuit is shown in Fig. 5.11(a). Figure 5.10 shows the pinch-off characteristics of QPC-defined quantum wires in device Zn5-1A. The gates are defined at around $-13$ V, and the quantum wire pinches off at $-26$ V. In Fig. 5.10(b), leakage through the 30 nm-thick Al$_2$O$_3$ insulating layer begins to increase at around $V_{SG} = -20$ V, and reaches a few hundred nA at $V_{SG} = -30$ V. In device Zn5-1A with six quantum wires, half of the wires cannot be pinched off, and strong leakage is observed. Random defects in the Al$_2$O$_3$ layer and the large electric field are the main reasons for the leakage. Close to pinch-off, Coulomb-blockade oscillations are revealed, as seen in the inset of Fig. 5.10(a). The main limitation of the two-terminal measurements here is the large contact resistance in

Figure 5.11: Two-terminal (a) and four-terminal (b) measurement circuits. The different resistor is for different excitation voltage. The circuit (b) is used for measurements in a dilution fridge with an excitation voltage of 10 $\mu$V.
Ohmic contacts (around 1-2 kΩ). To observe quantised conductance, we have to perform a series-resistance correction. Even then, we still cannot observe quantised conductance at $T = 4$ K.

<table>
<thead>
<tr>
<th>Device</th>
<th>$d$ (nm)</th>
<th>$n_{2D}$ (cm$^{-2}$)</th>
<th>Insulator</th>
<th>$V_{\text{def}}$ (V)</th>
<th>Model (V)</th>
<th>Leakage</th>
</tr>
</thead>
<tbody>
<tr>
<td>Zn5-1A</td>
<td>500+30</td>
<td>$3.1 \times 10^{12}$</td>
<td>Al$_2$O$_3$</td>
<td>-12</td>
<td>-12</td>
<td>x</td>
</tr>
<tr>
<td>Zn5-2A</td>
<td>500+30</td>
<td>$1.1 \times 10^{11}$</td>
<td>Al$_2$O$_3$</td>
<td>-11</td>
<td>-3.4</td>
<td>√</td>
</tr>
<tr>
<td>Zn5-2B</td>
<td>500+40</td>
<td>$3.1 \times 10^{11}$</td>
<td>parylene-$C$</td>
<td>-4</td>
<td>-3.4</td>
<td>x</td>
</tr>
<tr>
<td>Zn1-1A</td>
<td>92+30</td>
<td>$3.7 \times 10^{11}$</td>
<td>Al$_2$O$_3$</td>
<td>-8</td>
<td>-1</td>
<td>√</td>
</tr>
<tr>
<td>Zn1-1B</td>
<td>92+40</td>
<td>$3.7 \times 10^{11}$</td>
<td>parylene-$C$</td>
<td>-1.5</td>
<td>-1.2</td>
<td>x</td>
</tr>
</tbody>
</table>

Table 5.2: Comparisons of gate definition voltages in different devices with different insulators.

Using the quantum capacitor model, the gate definition voltage can be calculated from dielectric constant, dielectric layer thickness, and 2DEG density

$$\frac{V_{SG} - V_F}{d} = E = e \frac{n_{2D}}{\varepsilon \varepsilon_0},$$

where $V_F = E_F/e$, $E_F$ is the Fermi energy, and is small enough to be ignored compared to $V_{SG}$; $d$ is the thickness of the MgZnO layer, and $\varepsilon$ is the dielectric constant of the MgZnO layer, which is around 8.3. In device Zn5-1A, $n_{2D} = 1.2 \times 10^{12}$ cm$^{-2}$, the thickness of the MgZnO layer is 500 nm and the dielectric constant is 8.3. The calculated definition voltage of the gate matches the experimental results. In device Zn5-2A, the electron density is reduced to $n_{2D} = 3 \times 10^{11}$ cm$^{-2}$, so the definition voltage should also decrease to $-3.4$ V. However, with an Al$_2$O$_3$ insulator, the definition voltage is still around $-12$ V, which cannot be explained by the capacitor model,
as shown in Fig. 5.12(a). Figure 5.12(b) shows that when parylene-C replaces the Al$_2$O$_3$, the gate definition appears at $-4 \text{ V}$, matching the capacitor model. We also observe a similar effect in devices with a shallow 2DEG. With an Al$_2$O$_3$ insulator, the definition voltage is around $-8 \text{ V}$ in device Zn1-1A with $n_{2D} = 3.3 \times 10^{11} \text{ cm}^{-2}$. However with a parylene-C insulator, the gate is defined at $-1.5 \text{ V}$ in device Zn1-1B, as shown in Figs. 5.12(c) and (d). Table 5.2 compares the definition voltage of gates in different devices. From these measurements, we find that the devices with a low-density 2DEG are more easily damaged by the Al$_2$O$_3$ insulator than those with a high-density 2DEG. However, the parylene-C insulator works very well for devices with a low-density 2DEG. Up to now, we have not fully understood this damage.

5.3.2 Quantum Hall measurements

![Circuit Diagram](image_url)

Figure 5.13: Measurement circuit for quantum-Hall measurement

The quantum Hall measurement is an important method to assess a 2DEG in a heterostructure. Proper quantum Hall measurements need a low temperature, and therefore we perform these experiments in a $^3\text{He}/^4\text{He}$ dilution fridge with a base temperature at around 50 mK. In the refrigerator, the cooling process uses a mixture of $^3\text{He}/^4\text{He}$ with a ratio around 6.6% to 93.4%. At below 800 mK, the phase separation of $^3\text{He}$ and $^4\text{He}$ creates a $^3\text{He}$-rich phase or concentrated phase, which $^3\text{He}$ is in a superfluid of $^4\text{He}$. High energy $^3\text{He}$ atoms ‘boil off’ from the $^3\text{He}$ layer into the diluted phase, taking energy with it, so a $^3\text{He}/^4\text{He}$ dilution fridge can cool a sample down to 10 mK.

Figure 5.13 demonstrates the circuit for the quantum-Hall measurement. We apply an AC bias of 1 V oscillating at a frequency of 77 Hz to a large resistor (10 MΩ), which is in series with the device. Because of this large resistor, the change in 2DEG resistance has a negligible effect, and there should be a constant current of 100 nA. The 2DEG resistance, $R_{xx}$, and Hall resistance, $R_{xy}$, are measured with two lock-in amplifiers. As shown in Fig. 5.14 (b), when sweeping an out-of-plane magnetic field, $B$, $R_{xx}$ begins to oscillate, which is well-known as the Shubnikov–de-Hass (SdH) effect. At around 0.5 T, the peaks begins to split due to the Zeeman effect. In the Fourier transform, the spin-split and non-spin-split peaks are clearly shown at 14 T and 7 T, as seen in inset of Fig. 5.14(b). From the period of the oscillation, $n_{2D}$ is
deduced from Eqn. 5.12.

\[ \Delta \left( \frac{1}{B} \right) = \frac{1}{B_{i+1}} - \frac{1}{B_i} = \frac{2e}{n_{2D} h} \]  

(5.12)

where \( i \) is the index of the oscillation peak. If the oscillation peak is spin-polarised, the factor of 2 should be removed. As \( B \) increases, \( R_{xy} \) increases linearly. When \( R_{xx} \) reaches the minimum, \( R_{xy} \) becomes the quantum Hall plateau at \( h/\nu e^2 \), where \( \nu \) is the Landau-level filling factor. From \( n_{2D} \) and \( R_{xx} \) at zero field, the electron mobility is estimated by

\[ \mu = \frac{\sigma}{e n_{2D}} = \frac{1}{e R_{xx} n_{2D} L W}, \]  

(5.13)

where \( L \) and \( W \) is dimensions of the Hall bar.

Figure 5.14: Quantum-Hall measurement of the devices with different insulators: (a) Al\(_2\)O\(_3\), (b) parylene-C, at fridge base temperature of 50 mk. Inset in (b): fast Fourier transform of \( R_{xx} \) vs. \( 1/B \) with spin-split and no-split peaks.

We compare the quantum-Hall results in devices with different insulators. Figure 5.14(a) shows an abnormal quantum Hall result in device Zn1-1A with an Al\(_2\)O\(_3\) insulator. As \( B \) increases, both \( R_{xx} \) and \( R_{xy} \) increase linearly, which indicates that there may be strong parallel conduction in addition to the 2DEG. Probably this conducting layer forms at the Al\(_2\)O\(_3\)/ZnO interface, which might be interesting and worthwhile for further investigation. SdH oscillations are still observed. From the period of oscillations, \( n_{2D} \) matches the 2DEG density without an insulator. Figure 5.14(b) shows the quantum-Hall result in device Zn1-1B with parylene-C insulator; even though there is still weak parallel conduction, the quantum-Hall result is
significantly improved. Later, we compared the quantum Hall result for the device in the wafer Zn1-1 with and without a parylene-C insulator and observed similar SdH oscillations. This result indicates that the parylene-C insulator is not the reason for the parallel conduction. The ion-milling process may also damage the 2DEG, and this has not yet been fully explained, probably from the ion bombardment. Moreover, we can still see fractional quantum-Hall plateaus at $\nu = 5/3$ and $4/3$, which is an important sign of a good-quality 2DEG after the parylene-C deposition.

Figure 5.15: Temperature dependence of SdH oscillations from $T = 0.4$ to 1.2 K. The inset shows the fitting of $\ln(\Delta R_{xx}/T)$ as a function of $T$ at fixed magnetic fields, and $m^*$ is estimated to be $0.36 \pm 0.02 m_e$.

The SdH oscillation is strongly temperature-dependent. As the temperature increases, the SdH oscillation is damped. The amplitude of SdH oscillation, $\Delta R_{xx}$, can be fitted the Dingle expression

$$\Delta R_{xx} \propto \frac{\chi}{\sinh \chi} e^{-\pi/(\omega_c \tau_q)},$$

where $\chi = 2\pi^2 k_B T/(\hbar \omega_c)$, $\omega_c = eB/m^*$, $\tau_q$ is the quantum scattering lifetime (which we assume is temperature-independent over this measurement range) and $T$ is the temperature. The electron effective mass, $m^*$, obtained from this fit is around $0.36 \pm 0.02 m_e$ in this MgZnO/ZnO heterostructure, higher than it is in bulk ZnO (around $0.3 m_e$), where $m_e$ is the bare electron mass. The detailed explanation for the larger $m^*$ is discussed later.

In the dilution fridge MX40, we find a hysteresis in the shape of the SdH oscillations when sweeping $B$ in opposite directions. The SdH oscillations for sweeping $B$ from 0 to 2 T are different from those when $B$ sweeps from 2 T to 0, as shown in Fig. 5.16. The measurement with $B$ sweeping towards to zero shows a higher SdH oscillation amplitude than when sweeping away from zero. The amplitude when $B$ sweeps away from zero at 500 mK is roughly the same as when sweeping towards zero at 700 mK. This result shows that there is around 100-200 mK of heating when $B$ sweeps away from zero.

In an adiabatic process, the total energy is conserved. According to the quantum caloric effect, when a magnetic field is swept away from zero, magnetic dipoles
in a ferromagnetic substrate become aligned, decreasing magnetic entropy and heat capacity, and hence the substrate heats up. When the magnetic field is swept back to zero, the magnetic dipoles become randomly orientated and the magnetic entropy increases, taking heat from the environment, and hence cooling down the substrate. This quantum caloric effect is usually observed in ferromagnetic materials. In this MgZnO/ZnO heterostructure, there are no intentional ferromagnetic dopants. However, there are low-density background dopants, such as Ni and Co, during MBE growth, resulting in the paramagnetic or diluted ferromagnetic properties observed previously. Moreover, there is also a possibility that there may be a ferromagnetic component in the MX40 dilution fridge, separate from the sample.

To confirm this, we measured the same device in another fridge, and this hysteresis was highly suppressed. This test proves that the caloric heating effect is from the fridge, not the device. Therefore, in the MX40 fridge, we only consider results from sweeping $B$ towards zero, not those away from zero. Moreover, we reduce the sweeping rate to 1 T/hr. Once $B$ is swept slowly enough, the cooling power is strong enough to cool the device back to base temperature quickly.

5.4 Results and Discussions

5.4.1 One-dimensional ballistic electron transport

In device Zn1-1B, we perform four-terminal measurements at a base temperature of 50 mK, as shown in Fig. 5.11(b). To minimise electron heating, we use a small excitation voltage of 10 $\mu$V, making $eV << kT$. Separate voltages are applied to each QPC using two Yokogawa GS200 DC voltage sources. Beyond the gate definition at around $-1.5$ V, as $V_{SG}$ sweeps in a more negative direction, the 1D quantised conductance, $G$, appears with plateaus in units of about $\Delta G = 2e^2/h$. 

Figure 5.16: $R_{xx}$ as a function of $B$ from 2 to $-2$ T (black lines) and -2 to 2 T (red lines) at different temperatures from 0.4 K to 1.2 K. These temperatures are read from a RuO$_2$ thermometer in the mixing chamber and are not necessarily the same as the electron temperature.
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Figure 5.17: Schematic diagram of diffusing and ballistic electron transport in a 1D wire with length $L$ and width $W$. $l_e$ is the electron mean free path. Figure from Ref. 142.

Figure 5.18: (a) Quantised conductance of wires A and B in device Zn1-1B. Inset: pinch-off characteristics of wire B. (b) $G$ as a function of split-gate voltage $V_{SG}$ for wire B, as the temperature is increased from 0.05 K to 0.9 K (from left to right, the red line indicates data obtained at the fridge base temperature of 0.05 K, and the black lines are for $T$ from 0.1 K to 0.9 K in steps of 0.1 K). Traces are offset to the right for clarity.
Both wires in device Zn1-1B are apparent up to $14e^2/h$ (two quantum wires with same dimensions of width $W = 300\,\text{nm}$ and length $L = 200\,\text{nm}$), as shown in Fig. 5.18(a). The electron mean free path $l_e = \sqrt{2\pi n_{2D} \hbar \mu / e}$ is around $3.2\,\mu\text{m}$ in the MgZnO/ZnO heterostructure (Zn1-1), where $\mu$ is the mobility and $n_{2D}$ is 2DEG density. This $l_e$ is much larger than the device dimensions and so ballistic transport is possible, as shown in Fig. 5.17. At low conductance ($G < 2e^2/h$), Coulomb-blockade (CB) peaks appear because of the possible formation of dots owing to reduced electron screening and disorders. Since these oscillations obscure the first plateau, we will discuss results from the second plateau and above. At high conductance, other conductance features appear between the quantised plateaus. We will discuss these 0.7-like features in a later section. Figure 5.18 (b) shows the temperature dependence of $G$ as a function of split-gate voltage, $V_{SG}$, for wire B in device Zn1-1B. The step-like features in conductance are thermally smeared with increasing temperature. The quantised plateaus almost disappear at $T = 0.9\,\text{K}$.

The 1D quantised conductance is calibrated with a series resistance $R_s$:

$$G = \frac{1}{(1/G_m - R_s)}.$$  \hspace{1cm} (5.15)

Usually, we measure $R_s$ at $V_{SG} = 0$, which is around $110\,\Omega$. Even with calibration we still find the quantised plateaus do not match the $G = N \times 2e^2/h$, where $N = 1, 2, 3, \cdots$ is the 1D subband index, especially for the low subband. Data are corrected for a constant series resistance ($R_s = 110\,\Omega$) measured at $V_{SG} = 0$. This resistance does not lead to a constant vertical spacing of $2e^2/h$ between plateaus. Instead, the spacing is less than $2e^2/h$ near pinch-off and increases to close to $2e^2/h$ as $G$ increases, as shown in Fig. 5.18. This indicates that $R_s$ increases as $G$ decreases. The correction overestimates the voltage drop across the device and underestimates the conductance for lower subband indices. Therefore, this simple correction cannot align all the quantised plateaus with exact integer multiples of $2e^2/h$. The region near the wire will be affected by $V_{SG}$. Its series resistance will increase as $V_{SG}$ becomes more negative, reducing the electron density and hence the elastic mean free path, $l_e$, because of reduced screening. $l_e$ is lower than in GaAs because of the higher effective mass and it may become short enough for collisions with impurities to occur within the region affected by the gate, causing the series resistance to change more than it does for electrons in GaAs. It is therefore likely that the apparent suppression of the $4e^2/h$ plateau is a result of incorrect series resistance, and the plateau should be closer to $4e^2/h$. Moreover, $l_e$ decreases as temperature increases, and this is likely to increase further near the channel, as seen in Fig. 5.18(b).

The CB peaks at low conductance are presumably due to the impurities in the quasi-1D wire. These impurities become scattering centres and affect the ballistic electron transport. By applying an asymmetric bias, the position of the quasi-1D wire is shifted to avoid the impurities. Figure 5.19 shows the asymmetric-bias measurement in device Zn1-1B. We apply an asymmetry voltage $\Delta V_{SG} = V_{SG1} - V_{SG2}$ from $0.5\,\text{V}$ to $-0.5\,\text{V}$ on the QPCs, and find that the conductance plateaus stay in the same positions, indicating the conductance plateaus are largely impurity-independent. The CB peaks evolve significantly with asymmetric bias, which clearly distinguishes from the 1D conductance plateaus, as shown in Fig. 5.19.

When a DC bias is applied to one of the Ohmic contacts, the energy spacing between 1D subbands is probed. Figure 5.20 shows DC-bias spectroscopy of wires A
Section 5.4. Results and Discussions

Figure 5.19: Conductance $G$ as function of $V_{SG1}$ as an asymmetric bias is applied to the gates of wire B. The difference in voltage on the two split gates is defined by $\Delta V_{SG} = V_{SG1} - V_{SG2}$ changes from 0.5 V to $-0.5$ V in steps of 50 mV.

Figure 5.20: Transconductance $dG/dV_{SG}$ as a function of DC bias ($V_{DC}$) and $V_{SG}$ for wires A and B in device Zn1-1B. Dark/bright regions correspond to plateaus/risers in conductance. The energy difference between the third and fourth 1D subbands is indicated by $e\Delta V_{DC}$ in the plot. The numbers indicate the heights of quantised conductance plateaus in units of $e^2/h$. 

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and B. The colour scale shows the transconductance $dG/dV_{SG}$, such that dark/light regions correspond to plateaus/transition between plateaus. The splitting of the source and drain Fermi levels induced by the DC bias drives the evolution of quantised plateaus to odd-integer values, $G = Me^2/h$, where $M = 3, 5, 7, \cdots$, resulting in the diamond-shaped features in Fig. 5.20. The 1D subband energy spacing ($\Delta E$) is given by the height of the diamond multiplied by $e$ and is around 0.04 meV for the channel. This remains reasonably constant as the 1D subband index increases. The DC-bias dependence below $G = 2e^2/h$ is not clear, so we cannot comment about the 0.25 and 0.85 features that are commonly observed in GaAs wires, which have been attributed to spin polarisation. Because of the relatively small 1D subband spacing, the quantised plateaus in the MgZnO/ZnO heterostructure are strongly temperature dependent. As the temperature increases, the quantised conductance is highly degraded, and disappears for $T = 0.9$ K, as shown in Figure 5.18(b). Except the impurities in the 1D wire, lines such as the nearly horizontal line at $V_{SG} = -2.9$ V in Fig. 5.20 (wire A) or near $V_{SG} = -2.6$ V (wire B) must come from a random impurity or dot, perhaps under a gate, as they are only very slightly dependent on $B$ or $V_{DC}$ and so must provide a conduction path in parallel to the 1D wire.

![Figure 5.21](image-url)

**Figure 5.21:** Conductance as a function of $V_{SG1}$ as an asymmetric bias is applied to the QPCs for the wire C in device Zn5-1A. The asymmetric bias $\Delta V_{SG}$ changes from 5 V to −5 V in steps of 0.1 V, where $\Delta V_{SG} = V_{SG1} - V_{SG2}$.

The 1D quantised conductance is strongly dependent on the dimension of the QPCs. We fabricate wire C in device Zn5-1A with a length of 300 nm and a width of 800 nm. In device Zn5-1A, the 2DEG is located 500 nm below the surface. Fringing
Figure 5.22: Transconductance \( dG/dV_{SG1} \) with asymmetric bias on QPCs (the dark regions indicate quantised plateaus and the light regions indicate the transitions between plateaus). \( V_{SG1} \) is swept at a fixed \( V_{SG2} \), which is incremented from \(-15 \) V to \(-21 \) V. (b) Model of total quantised plateaus in two parallel 1D wires, controlled by \( V_{SG1} \) and \( V_{SG2} \).

fields expand and make the 1D wire much longer than 300 nm. In a longer 1D wire, impurities are more difficult to avoid. When the asymmetric bias is applied, the quantised plateaus are shifted, as shown in Fig. 5.21. There is another way to apply the asymmetric bias. We can sweep one gate voltage and leave the other gate voltage fixed. Figure 5.22(a) shows the measured transconductance \( dG/dV_{SG1} \) in wire C at various \( V_{SG2} \). Figure 5.22(b) demonstrates a model of quantised conductance in two parallel channels controlled by \( V_{SG1} \) and \( V_{SG2} \). The experimental results are similar to those of the model but more irregular. Due to the existence of random impurities, the 1D wires defined by QPCs may be split into several parallel wires for electron travelling. These multiple channels lead to a strong dependence on asymmetric bias for wire C in device Zn5-1A.

5.4.2 Zeeman splitting and enhanced \( g \)-factor

When an in-plane magnetic field is applied to a 1D wire, the electron energy splits due to the Zeeman effect. Here for a non-Rashba system, whether an in-plane magnetic field is aligned or perpendicular to the 1D wire does not matter. Figure 5.23(a) shows the differential conductance \( dG/dV_{SG} \) as a function of in-plane magnetic field, \( B_{\parallel} \) from 0 to 8 T in wire A. At \( B_{\parallel} = 0 \), quantised plateaus occur at even-number multiples of \( e^2/h \). At \( B_{\parallel} = 0.5 \) T quantised plateaus occur at \( G = ne^2/h \), where \( n = 3, 4, 5, \cdots \) due to Zeeman splitting, indicating the electron spins are fully resolved. As \( B_{\parallel} \) increases to 1 T, the spin-split 1D subbands cross and plateaus occur at \( G = Me^2/h \), where \( M = 3, 5, 7, \cdots \). As \( B_{\parallel} \) further increases, the electrons at lower subbands begin to become fully polarised, and independent of \( B_{\parallel} \), as with the red lines in Figure 5.23(a).

From the Zeeman energy and 1D subband spacing, we estimate the \( g \)-factor \((g^*)\) according to Eqn. 5.16

\[
|g^*| = \frac{1}{\mu_B} \frac{\delta E}{\delta V_{SG}} \frac{\delta V_{SG}}{\delta B} = \frac{e}{\mu_B} \frac{\Delta V_{DC}}{\Delta B},
\]  
(5.16)
where $e$ is the electric charge and $\mu_B$ is the Bohr magneton.\textsuperscript{143} In Table 5.3, we estimate $g^* \approx 6.8$ for the second 1D subband and 6.4 for the sixth. This is enhanced above the bulk value of around $g^* = 2$ for MgZnO/ZnO heterostructures and bulk ZnO.\textsuperscript{130} A similar, but smaller, enhancement of $|g^*|$ occurs for electrons in GaAs QPCs, for which studies have reported a range of values from 0.75 to 1.5 for 1D constrictions,\textsuperscript{59,147,148} compared to the bulk value of 0.44. The percentage increase compared to the bulk that we measure is within the range of that reported for GaAs. It has also been shown that $|g^*|$ decreases fairly rapidly with subband index for electrons in GaAs QPCs.\textsuperscript{149} However, in our data, $g^*$ is reasonably constant since the Zeeman splittings of 1D subbands as a function of $B_\parallel$, as seen in Fig. 5.23(b), are almost identical; the gradient of slopes representing 1D subband edges and the field at which adjacent spin-split subbands cross are very similar for 1D subbands 2 to 6, as shown in Table 5.3.

\begin{table}[h]
\centering
\begin{tabular}{|c|c|c|c|c|c|}
\hline
Subband index & 2 & 3 & 4 & 5 & 6 \\
\hline
$g^*$ & 6.8 & 6.8 & 6.4 & 6.1 & 6.4 \\
\hline
\end{tabular}
\caption{Enhanced $g^*$ at 1D subband indices 2 to 6.}
\end{table}

Figure 5.23: Transconductance $dG/dV_{SG}$ in a unit of $2e^2/h/V$ as a function of $V_{SG}$ and $B_\parallel$ in wires A (a) and B (b). The arrow and $\Delta B$ indicate the required $B_\parallel$ for the energy to cross of the subband $2^\uparrow$ and $3^\downarrow$. 

In Table 5.3, we estimate $g^* \approx 6.8$ for the second 1D subband and 6.4 for the sixth. This is enhanced above the bulk value of around $g^* = 2$ for MgZnO/ZnO heterostructures and bulk ZnO.\textsuperscript{130} A similar, but smaller, enhancement of $|g^*|$ occurs for electrons in GaAs QPCs, for which studies have reported a range of values from 0.75 to 1.5 for 1D constrictions,\textsuperscript{59,147,148} compared to the bulk value of 0.44. The percentage increase compared to the bulk that we measure is within the range of that reported for GaAs. It has also been shown that $|g^*|$ decreases fairly rapidly with subband index for electrons in GaAs QPCs.\textsuperscript{149} However, in our data, $g^*$ is reasonably constant since the Zeeman splittings of 1D subbands as a function of $B_\parallel$, as seen in Fig. 5.23(b), are almost identical; the gradient of slopes representing 1D subband edges and the field at which adjacent spin-split subbands cross are very similar for 1D subbands 2 to 6, as shown in Table 5.3.

<table>
<thead>
<tr>
<th>Subband index</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
</tr>
</thead>
<tbody>
<tr>
<td>$g^*$</td>
<td>6.8</td>
<td>6.8</td>
<td>6.4</td>
<td>6.1</td>
<td>6.4</td>
</tr>
</tbody>
</table>

Table 5.3: Enhanced $g^*$ at 1D subband indices 2 to 6.
5.4.3 Out-of-plane magnetic field measurements

Figure 5.24: Schematic diagram of Landau-level reflection and transmission with a QPC.

For a magnetic field, $B_\perp$, applied perpendicular to the 2DEG, the electron energy contains both the Zeeman ($E_z$) and cyclotron energy ($E_c$) terms:

$$E_N(B) = \left(N + \frac{1}{2}\right)\hbar\sqrt{\omega_0^2 + \omega_c^2} \pm \frac{1}{2}\frac{g^*\mu_B}{\omega_c},$$  \hspace{1cm} (5.17)

where $N$ is the 1D subband index, $\hbar\omega_0$ is the 1D subband spacing assuming a parabolic potential, and $\omega_c = eB_/m^*$ is the cyclotron frequency.$^{150}$

In an out-of-plane field, electron edge states are defined and reflected by QPCs, as seen in Fig. 5.24. To measure the transmitted edge states, we use the ‘diagonal’ measurement according to the Büttiker formula.$^{151}$ Current starts at the source, S, or leave at the drain, D. In the 2DEG, there are $N$ occupied Landau levels, and $N - M$ of those are reflected by QPC. So there are only $M$ Landau levels that are transmitted. By choosing different Ohmic probes, the different state of Landau levels are measured with $R_{ij}$, where $i$ and $j$ is the indices of the Ohmic probes in Fig. 5.24,

$$R_{13} = \frac{h}{N e^2},$$  \hspace{1cm} (5.18)

$$R_{14} = \frac{h}{M e^2},$$  \hspace{1cm} (5.19)

$$R_{12} = \left(\frac{1}{M} - \frac{1}{N}\right)\frac{h}{e^2}. \hspace{1cm} (5.20)$$

In our experiment, we use diagonally opposite probes 1 and 4 to measure $R_{14}$, giving the transmitted Landau levels.

Figures 5.25 (a) and (b) demonstrate the evolution of the conductance plateaus as a function of $B_\perp$ in device Zn5-1A. At $B_\perp = 0$, the conductance plateaus are not well defined. As $B_\perp$ increases, the quantised plateaus appear at $G = Me^2/h, M = 1, 3, 5, \ldots$. Then, as $B_\perp$ further increases, another set of plateaus is shown at even multiples of $e^2/h$. At around 1 T, we observe the odd-numbered quantised plateaus up to $31e^2/h$, as shown in Fig. 5.25(c). This effect is very different from the same
Figure 5.25: (a) Conductance as a function of $V_{SG}$ at different magnetic fields 0 to 8 T with an increment of 1 T. (b) Transconductance $dG/dV_{SG}$ as a function of $V_{SG}$ and $B_{\perp}$ from 0 to 10 T. There are two sets of Landau fans with a boundary at $V_{SG} = -12$ V. (c) Transconductance $dG/dV_{SG}$ as a function of $V_{SG}$ and $B_{\perp}$ in more details from 0 to 1.3 T. The labelled numbers indicate the heights of quantised conductance plateaus in units of $e^2/h$. 

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measurement in a GaAs wire, which involves even-numbered quantised plateaus. However, the quantised plateau at zero fields is not clear. We fail to observe how zero-field quantised plateaus evolve into these odd-numbered plateaus in device Zn5-1A.

In device Zn1-1B, however, we successfully observed this smooth evolution, as shown in Fig. 5.26. In the low-field regime ($\omega_0 \gg \omega_c$), the spin-degenerate plateaus at even multiples of $G = e^2/h$ are split by the Zeeman energy, leading to additional conductance plateaus at $G = ne^2/h$, where $n = 1, 2, 3, \cdots$. These merge to odd multiples of $G = e^2/h$ with increasing $B_\perp$ as adjacent spin-split 1D subbands cross. However, in the high $B_\perp$ regime, Landau-level formation leads to the creation of hybrid magneto-electric subbands in the constriction, for which plateaus again occur at both even and odd integers $G = ne^2/h$. The onset of this regime can be quantified by the ratio of the cyclotron and Zeeman energies, $\kappa = E_c/E_z = \hbar\omega_0/(g^*m^*\mu_B)$. We estimate that $m^* = (0.36 \pm 0.02)m_e$ for our ZnO heterostructure from temperature-dependent Shubnikov–de-Haas measurements and the Dingle formula, as seen in Figs. 5.15. This gives $\kappa < 1$ for $g^* = 6.8$. The smaller effective mass and $g$-factor in GaAs devices ($m^* = 0.067m_e$ and $|g^*| \approx 1$), lead to $\kappa \gg 1$, so that the regime with odd-integer conductance plateaus that occurs when adjacent spin-split 1D subbands cross is not observed.

Figures 5.26(a) and (b) show the evolution of the 1D subbands with $B_\perp$. Bright regions correspond to high transconductance $dG/dV_{SG}$ (risers in conductance between plateaus), where subband edges cross the Fermi energy. The plateau heights in different regions are labelled in Fig. 5.26(a) and (b). We model the 1D subband energy as a function of magnetic field using Eqn. 5.17. Results for constant $m^* = 0.4$, $g^*$ and $\hbar\omega_0$ are plotted in Fig. 5.26(c). Black and red lines represent spin-down ($\downarrow$) and spin-up ($\uparrow$) subbands, respectively. The evolution of plateaus matches the experimental data. However, the value of $B_\perp$ at which 1D subbands cross is independent of subband index, which does not match the measurements. In Fig. 5.26(a), the crossing between $N = 2\uparrow$ and $N = 3\downarrow$ occurs around $B_\perp = 0.8$ T, and that between $N = 3\uparrow$ and $N = 4\downarrow$ occurs around $B_\perp = 1.2$ T. For the higher subbands $N > 4$, the required $B_\perp$ for subband crossing decreases.

Motivated by previous reports that $m^*$ in ZnO electron systems increases as the density reduces, we repeat the calculation with $m^*$ increasing from 0.4 to 1 as the 1D subband index decreases, plotted in Fig. 5.26(d). This qualitatively reproduces the trend from experimental data that the value of $B_\perp$ at which spin-split subbands cross initially increases, then decreases for higher subbands (although the model tends to overestimate the values of $B_\perp$, or the crossing points in experiments are underestimated due to energy blurring). We choose to vary $m^*$ instead of $g^*$ since our data suggest that $g^*$ is reasonably constant as a function of the subband index, unlike in GaAs. Also, the DC-bias spectroscopy measurement in Fig. 5.20 indicates that the 1D subband spacing is also reasonably constant over this range.

In the experiments, the precise points at which the bands cross at low subband index cannot be determined, and some look more like anticrossings (labelled $\gamma$ in Fig. 5.26(a)). This may occur because of a strong electron-electron interaction, and could be modelled by introducing an exchange interaction term in Eqn. 5.17.

Figure 5.25(b) shows the transconductance $dG/dV_{SG}$ as a function of $V_{SG}$ from $-8$ to $-19$ V. Two independent Landau fans are observed. One converges at $V_{SG} = -8$ V.
Chapter 5. Quantised conductance of 1D strongly-correlated electrons in a ZnO heterostructure

Figure 5.26: (a) (b) Transconductance $dG/dV_{SG}$ as a function of $V_{SG}$ and $B_\perp$ from 0 to 2.5 T for the wires A (a) and B (b) in device Zn1-1B. The ellipses or $\gamma$ indicate the energy level crossings or anti-crossings. (c) (d) Electron energy spectrum calculated as a function of $B_\perp$ with (c) constant and (d) increasing $m^*$. The numbers indicate the heights of quantised conductance plateaus in units of $e^2/h$, and blue dots mark the positions of 1D subband crossings.
Section 5.4. Results and Discussions

−12 V, and the other at \( V = -18 \) V. When \( V_{SG} > -12 \) V, electrons underneath the QPCs are not fully depleted, allowing for conduction beneath the gate. Therefore the two Landau fans come from the electrons travelling underneath and between the gates, as shown in Fig. 5.27. Electrons between and beneath gates behave differently in magnetic fields. The odd-dominated effect is more obvious between the gates than it is beneath the QPCs. Underneath the gates, the electrons are more two-dimensional, and the electrons between gates are quasi-one-dimensional. This reduction in dimensionality contributes to the enhancement of \( m^*g^* \), which plays an essential role in this odd-even evolution of the conductance plateaus.

![Figure 5.27: Two types of electron paths through a gate.](image)

5.4.4 Strongly-correlated electrons and enhanced \( m^* \)

To further investigate \( m^* \) we measure the DC-bias dependence for wire A in device Zn1-1B at \( B_\perp = 1 \) T, as shown in Fig. 5.28(a). Adjacent spin-split subbands cross near \( B_\perp = 1 \) T, as indicated by only odd plateaus being present in the conductance trace for \( V_{DC} = 0 \). Since the 1D subband spacing is roughly constant, each pair of subbands \( 2\uparrow/3\downarrow, 3\uparrow/4\downarrow \), etc. is degenerate since spin\( \uparrow/\downarrow \) subbands are shifted by \(+/- g\mu_B B\), respectively, cancelling out the Zeeman term. The energy difference between these pairs of subbands is therefore

\[
\Delta E = \hbar \sqrt{\omega_0^2 + \omega_c^2}.
\] (5.21)

In contrast with the \( B_\perp = 0 \) case, Fig. 5.28(a) shows that at \( B_\perp = 1 \) T the spacing between the subband pairs is lower for a lower subband index \( N \). This could be explained by an increase in \( m^* \), leading to a smaller cyclotron energy \( E_c = \hbar eB/m^* \) for a lower \( N \). Figure 5.28 (b) shows the measurement repeated for device C, in which more plateaus are evident. This uses another MgZnO/ZnO heterostructure with a higher 2DEG density, \( n_{2D} = 1.2 \times 10^{12} \) cm\(^{-2}\), for which the crossing of spin-split subbands occurred at \( B_\perp = 2 \) T. The same trend of increasing spacing with subband index occurs. (All DC-bias data are corrected for series resistance using

\[
V_{DC} = V_{DC}^{appl} (1 - R_S \int_0^{V_D} GdV_{DC}),
\] (5.22)

where \( R_S \) is the series resistance measured at zero gate voltage, and \( V_{SD}^{appl} \) is the DC bias applied in the measurement.\(^{156}\)
Figure 5.28: Transconductance $dG/dV_{SG}$ as a function of $V_{SG}$ and DC bias $V_{DC}$ for wire A (a) in device Zn1-1B at $B_{\perp} = 1$ T, and wire C (b) in device Zn5-1A at $B_{\perp} = 2$ T. In device Zn5-1A, the high electron density and thick MgZnO (500 nm) require strong negative voltages to define the 1D wire. The conductance values of the quantised plateaus are indicated in units of $e^2/h$. (c) The measured $m^*$ as a function of $G$ in both devices, and compared with the bulk value for ZnO.
Figure 5.28(c) shows the estimated \( m^* \) as a function of the conductance plateau height (in units of \( e^2/h \)), estimated using Eqn. 5.21. At high conductance, \( m^* = (0.31 \pm 0.03) \, m_e \), close to the bulk effective mass in ZnO. When \( G \) decreases to \( 5e^2/h \), \( m^* \) increases to \( m^* = 0.96 \pm 0.2 \, m_e \). The large error bar is due to the blurred nature of this 1D subband crossing. However, the trend for effective mass to increase as conductance decreases is clear. This represents a significant difference from GaAs QPCs in which \( m^* \) is roughly constant.

In previous studies of MgZnO/ZnO heterostructures, \( m^* \) measured by \( T \)-dependent SdH oscillations increases as the 2DEG density decreases, while \( m^* \) measured using cyclotron resonance is roughly constant.\textsuperscript{125,153} This indicates that the increase in the transport effective mass arises from electron-electron interactions, which are more significant at lower density. A similar effect is also observed in Al-GaAs/GaAs heterostructures,\textsuperscript{126} but it is much weaker. Here, our measurements of \( m^* \) in 1D transport in ZnO heterostructures show a similar trend—the electron-electron interaction strength is stronger than in GaAs owing to the larger \( r_S \) arising from the higher effective mass, and \( r_S \) increases as the subband index decreases, both through reduced density and increased mass.

5.4.5 N.7 anomalies

![Figure 5.29: 0.7 anomaly in a GaAs quantum wire and its evolution in an in-plane magnetic field from 0 to 13 T. Figure from Ref. 59.](image)

An anomalous feature at \( G = 0.7 \times 2e^2/h \) was first investigated by Thomas et al.\textsuperscript{59} They found that as the in-plane magnetic field increases, the 0.7 plateau smoothly evolves into a 0.5 plateau, indicating a possible spontaneous spin polarisation, as shown in Fig. 5.29.\textsuperscript{59,157} The origin of this has since been much debated,\textsuperscript{158} and various other theories have been proposed including quasi-bound state formation and the Kondo effect.\textsuperscript{159,160} Recently, Bauer et al. have used the smeared van...
Hove singularity to explain its occurrence and have emphasised the important role that electron-electron interactions play in the 0.7 anomaly.\textsuperscript{161}

We now return to our discussion of the 0.7 anomaly. Figure 5.18(a) shows several shoulder-like features below the main quantised plateaus up to the fifth 1D subband. We perform several measurements to test whether they behave similarly to the 0.7 anomaly or CB-like resonances from impurities.

- i) Resonant peaks from CB should split with $V_{\text{DC}}$ at a rate determined by the size of the dot-like impurity and coupling to the gates. The DC-bias spectroscopy for our devices shows an orderly splitting above the second plateau typical of clean 1D devices,\textsuperscript{146,163} as seen in Fig. 5.20. Below the first plateau, the splitting of CB-like peaks has a very different gradient compared to the 1D subband splitting, because of the different energy scales. Above the second plateau, there is no further evidence of splitting with markedly different gradients, indicating no further CB oscillations.

- ii) In Figures 5.23(a) and (b), even a small magnetic field is enough to lift spin-degeneracy. The lines of high transconductance indicating the edges of spin-split subbands do not converge at $B = 0$, showing clear gaps [for example, $\beta_0$, $\eta_0$, and $\delta_0$ in Fig. 5.30(b)] at the quantised plateaus, which have also been seen for the 0.7 anomaly in GaAs.\textsuperscript{59} Fig. 5.30(b) also shows gaps at higher-order crossings (labelled $\alpha_2$, $\beta_1$, $\beta_2$, $\eta_1$ and $\delta_1$ matching the labels in Fig. 5.30(a)), which is an important sign of the 0.7 analogue.\textsuperscript{162} The gaps can be explained as an effect of electron-electron interactions.\textsuperscript{164} Compared to the 0.7 anomaly in a GaAs quantum wire, the N.7 analogues in this ZnO quantum wire are much clearer and stronger, which is probably related to the strong electron-electron interaction.

- iii) The conductance sweeps in Fig. 5.30(c) are re-plotted in Fig. 5.30(d) as lines for fields from $B_{\parallel} = 0$ to 1 T. The N.7 plateaus (near $G = 2Ne^2/h$) appear to evolve smoothly to spin-polarised plateaus at $G = (N - 1/2)2e^2/h$, then split (also indicated as * and white dashed lines in Fig. 5.30(c) and (d)). This split before the crossing was also observed in GaAs, but was much weaker than it is here in ZnO, as shown in Fig. 5.30 (b).\textsuperscript{162} Moreover, we find that the gap is so large that the N.7 analogues almost connect, as shown by the white curves in Fig. 5.30(c). This feature has never been observed before in a GaAs quantum wire. How electron-electron interactions contribute to this feature needs further theoretical investigation.

- iv) The quantised plateaus and N.7 structures stay reasonably constant as the wire is shifted laterally by an asymmetric bias on the QPC gates, as shown in Fig. 5.19. In contrast, the resonant peaks due to CB below the first plateau vary significantly. Coulomb-blockade-type features are not independent of position since the disorder potential changes as the wire moves relative to impurities. However, the wire position should not significantly affect either 1D quantisation or interaction effects inherent in the 1D system such as the 0.7 structure. However, small variations can occur if the asymmetry alters the wave-function localisation and therefore affects the strength of electron interactions and hence the 0.7 structure.\textsuperscript{161}
Figure 5.30: Transconductance, \( dG/dV_{SG} \), as a function of gate voltage and in-plane field in a GaAs wire. The 0.7 analogues are labelled, \( \alpha, \beta \) and *. Figures from Ref. 162. (c) Transconductance, \( dG/dV_{SG} \), as a function of \( V_{SG} \) in parallel magnetic fields \( B_{||} \) from 0-3 T in device Zn1-1B. The N.7 analogues are labelled \( \alpha, \beta, \delta, \eta \) and * to match (b). (d) Conductance as a function of \( V_{SG} \) at different \( B_{||} \) from 0 to 1 T in steps of 0.02 T. Each trace is shifted successively by 0.01 V for clarity. The red dots illustrate how the shoulder features resembling the 0.7 anomaly evolve with \( B_{||} \). ((c) and (d) use the same measurement data.)
Figure 5.31: (a) Temperature-dependence of the $0.7$ anomaly in a GaAs quantum wire. Figure from Ref. 59. (b) Temperature-dependence of the $N.7$ structure in a ZnO quantum wire from 0.05 T to 0.9 K. The blue filled circles indicate the evolution of the second 1D plateau at $G = 4e^2/h$, and the blue circles indicate the evolution of the 1.7 structure.

- v) The $0.7$ structure depends strongly on temperature. In a GaAs quantum wire, as the temperature increases, the $0.7$ plateau becomes flatter, and the 1D quantised plateaus degrade, as shown in Fig. 5.31(a). In a ZnO quantum wire, as mentioned before, the series resistance increases as the temperature increases, which makes temperature-dependent studies harder than in GaAs. Ignoring the uncertainties in series-resistance calibration, the second plateau ($N = 2$) degrades much faster than the ‘1.7’ structure, which is consistent with the behaviour of the 0.7 structure in GaAs, as shown by the arrows and blue dots in Fig. 5.31 (b). Because of the small 1D subband spacing in our samples, any structure is rapidly smeared out as the temperature is raised, disappearing entirely by $T > 1$ K. A potential solution is to measure devices with larger subband spacing, increasing the confinement strength by narrowing the lithographic width of the channel.

The strength of electron-electron interactions plays an essential role in the 0.7 anomaly, which becomes more pronounced as the interaction strength increases. In Fig. 5.18(a) and Fig. 5.30(d), the $N.7$ structures become progressively stronger and occur at a lower point on the riser for lower 1D subbands. This is consistent with stronger electron-electron interactions. The strongly correlated electron system in MgZnO/ZnO heterostructures offers a novel platform to investigate electron-electron interaction effects, in particular, the 0.7 structure. These strong correlations arise from the large effective mass and small dielectric constant $\varepsilon = 8.3$ compared to GaAs heterostructures. In a MgZnO heterostructure with a low-density 2DEG, $r_s$ can reach 10. In this 1D wire, the density can be even lower, and so the interaction can be even stronger. However, in a 1D system, we cannot use $r_s$ to represent the electron-electron interaction strength. These strong interactions may be the source of $N.7$ structures in 1D subbands with a higher index $N$ apparent in our data, which behave in a manner consistent with the 0.7 structure. Such $N.7$ structures are not often seen or are extremely weak in GaAs electron or hole systems,
since the interaction strength is weakened in higher 1D subbands.\textsuperscript{149,166–168} This MgZnO/ZnO heterostructure also shows dilute ferromagnetic properties and the anomalous Hall effect is observed.\textsuperscript{141} This usually results from spin-dependent electron scattering off localised magnetic moments, which are likely to arise from point defects in epitaxial ZnO with localised unpaired electrons.\textsuperscript{141} We also measure the magnetic moment at $T = 1.8\, \text{K}$ using a vibrating-sample magnetometer in conjunction with Mr Cheng Liu and Mr Chao Yun at the Quantum Matter group and the Department of Material. Figure 5.32 demonstrate the magnetic hysteresis near zero field, which also indicates the dilute ferromagnetic properties in the MgZnO/ZnO heterostructure. This ferromagnetism may also increase the strength of the 0.7-like structure because this generally appears to be strongly related to spin.\textsuperscript{59,161,169} However, the dilute ferromagnetic moments cannot be strong enough to produce full spontaneous electron spin polarisation in the 1D wire, as only plateaus at even multiples of $e^2/h$ are observed at $B = 0$. Instead, the dilute ferromagnetism may possibly help to enhance the local spin susceptibility in the channel at $B = 0$,\textsuperscript{161} making it easier for interactions to give rise to the shoulders on each plateau.

![Figure 5.32: Magnetic moment, $M$, of a MgZnO/ZnO heterostructure.](image)

Figure 5.32: Magnetic moment, $M$, of a MgZnO/ZnO heterostructure. This measurement is performed using a vibrating-sample magnetometer at $T = 1.8\, \text{K}$. The applied magnetic field perpendicular to the 2DEG is swept from 0.5 T to $-0.5$ T and back to 0.5 T. The hysteresis near zero field demonstrates the diluted ferromagnetic properties of this MgZnO/ZnO heterostructure.

\section{5.5 Conclusion}

To conclude, we have shown ballistic electron transport with clear conductance quantisation in 1D quantum wires defined on a MgZnO/ZnO heterostructure. We also report an increasing effective mass at a lower density, which is consistent with measurements on 2D ZnO systems. Because of the large $g^*$ and $m^*$, a perpendicular magnetic field drives the system into the regime in which the Zeeman energy is greater than the cyclotron energy, leading to only odd plateaus appearing in conductance. At zero field we see evidence of 0.7-like anomalies up to the fifth subband.
Such structures are not commonly observed in GaAs, a key reason for which is probably the significantly higher electron-electron interaction strength in ZnO. These results show that this high-quality MgZnO/ZnO heterostructure could be a promising alternative to III-V semiconductors as a platform for quantum information and spintronic technologies. The success of gating this ZnO heterostructure also pave the way for SAW-based quantum technologies, exploiting the strong piezoelectricity of the material. This will be explored in the next chapter.
In Chapter 4 we have discussed ZnO-enhanced SAW-pumping in an AlGaAs/GaAs heterostructure using the HiTUS technique. In Chapter 5, we investigated low-dimensional transport in a MgZnO/ZnO heterostructure and observed clear quantised conductance in a QPC-defined quantum wire. All these results indicate that we can combine the SAW technique with a MgZnO/ZnO heterostructure. P. Leek et al. have studied the SAW propagation on a single-crystal bulk ZnO substrate and observed a strong SAW resonance and studied its temperature dependence. Here we investigate SAW modulation in a MgZnO/ZnO heterostructure. As well as the classic SAW-pumping effect, we find other carrier modulation from the SAW.

Figure 6.1: (a) Crystal structure of an O-faced ZnO with a parallelepiped lattice with lattice constants $a$ and $c$. (b) Schematic diagram of a MgZnO/ZnO heterostructure with sheet conductance $\sigma$ (red line). The spontaneous and piezoelectric polarisation directions are indicated with arrows.
6.1 Spontaneous and piezoelectric polarisation

In Chapter 5, we have introduced the fact that the polarisation mismatch between MgZnO and ZnO originating from spontaneous and piezoelectric contributions induces a 2DEG at the interface. Here we give a detailed explanation and calculation of the polarisation-induced 2DEG in a MgZnO/ZnO heterostructure.

In a wurtzite crystal, such as ZnO or GaN, spontaneous ($P_{SP}$) and piezoelectric ($P_{PE}$) polarisation are exhibited along the polar [0001] or [0001] orientation. The spontaneous polarisation comes from the intrinsic asymmetry of bonding in the equilibrium wurtzite crystal, and the piezoelectric polarisation comes from mechanical stress in the crystal. The orientation of $P_{SP}$ depends on the polar orientation. In a ZnO heterostructure, if the upper ZnO layer is Zn-faced [0001], the $P_{SP}$ points towards the substrate. If it is O-faced [0001], $P_{SP}$ points to the surface. The orientation of piezoelectric polarisation depends on the strain. $P_{SP}$ and $P_{PE}$ are in parallel in the case of a tensile-strained upper layer, and anti-parallel in the case of a compressive-strained upper layer. The sheet charge $\sigma$ is given by:

$$\sigma = [P_{SP}(\text{top}) + P_{PE}(\text{top})] - [P_{SP}(\text{bottom}) + P_{PE}(\text{bottom})]. \quad (6.1)$$

Figure 6.2: ZnO lattice constants $a$ and $c$ as a function of Mg content $x$ at Al$_2$O$_3$ and ZnO substrates. Figure from Ref. 171.

Here we use a MgZnO/ZnO heterostructure with a tensile-strained MgZnO layer on a relaxed ZnO layer, and the MgZnO is O-faced with a polar direction of [0001], as shown in Fig. 6.1. Because the ZnO layer is relaxed, $P_{PE}(\text{bottom}) = 0$, and the $\sigma$ reduces to

$$\sigma = [P_{SP}(\text{top}) + P_{PE}(\text{top})] - P_{SP}(\text{bottom}) \quad (6.2)$$

The $P_{PE}$ is calculated from the strain along different lattice axes using

$$P_{PE} = e_{31}(S_{xx} + S_{yy}) + e_{33}S_{zz}, \quad (6.3)$$

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where $e_{31}$ and $e_{33}$ are piezoelectric coefficients from the piezoelectric matrix. $S_{xx}$ and $S_{yy}$ are the in-plane strain, and $S_{zz}$ is the out-of-plane strain. In a ZnO substrate, the in-plane strain is isotropic, and $S_{xx}$ or $S_{yy}$ can be expressed as $\Delta a/a$, and $S_{zz}$ is $\Delta c/c$, where $a$ and $c$ are the lattice constants in the ZnO crystal. Then Eqn. 6.3 is then corrected

$$P_{PE} = 2e_{31}(\Delta a/a) + e_{33}(\Delta c/c).$$  \hspace{1cm} (6.4)

$P_{SP}$ is estimated from an empirical rule for wurtzite crystals. An internal parameter, $u$, is introduced and $P_{SP}$ is estimated from the point-charge model,

$$P_{SP} = \left[-8/(\sqrt{3}a^2)\right](u - 3/8),$$  \hspace{1cm} (6.5)

where $u = (1/3)(a/c)^2 + 1/4$. In an ideal wurtzite compound, the cation is located at the centre of the anion tetrahedron. Therefore $u = 3/8 = 0.375$ and $P_{SP} = 0$. In a real crystal, the tetrahedron is deformed, creating asymmetry in bonds and giving non-zero $P_{SP}$. $P_{SP}$ in ZnO is reported to be $-0.054$ C/m$^2$. Figure 6.3 shows the measured $u$ as a function of $(a/c)^2$ for different wurtzite compounds, and the value is slightly different from the model $u = (1/3)(a/c)^2 + 1/4$. We use the calibrated $u$ ($u = 0.36(a/c)^2 + 0.24$) in Eqn. 6.5.

By controlling the Mg content, $x$, in $\text{Mg}_x\text{Zn}_{1-x}\text{O}$, we can modulate both $P_{SP}$ and $P_{PE}$, and hence $\sigma$ as well. By controlling $x$, the lattice constants $a$ and $c$ can be adjusted. Figure 6.2 shows the lattice constant as a function of Mg content at ZnO and $\text{Al}_2\text{O}_3$ substrates. It was found that $c$ decreases as $x$ increases, and $a$ increases for a ZnO substrate but stays constant for an $\text{Al}_2\text{O}_3$ substrate as $x$ increases. The best fit line is $\Delta c = -0.069x$.\textsuperscript{171}

In Ref. 114, Tsukazaki et al. investigated $P_{SP}$ and $P_{PE}$ in units of C/m$^2$ as a function of the Mg content:

$$P_{PE}(x) = (1.98 \pm 0.28)(0.027x^2 + 0.0083x).$$  \hspace{1cm} (6.6)
Chapter 6. SAW modulation in a ZnO heterostructure

Figure 6.4: Simulated 2DEG density as a function of Mg content $x$. The negative density means charges are accumulated at the surface instead of the interface.

By fitting the experimental results, they estimated the spontaneous polarisation mismatch $\Delta P_{SP} = P_{SP}(x) - P_{SP}(0)^{114}$

$$\Delta P_{SP} = -0.17x^2 - 0.009x.$$ (6.7)

Finally the sheet charge density, $\sigma/e$, can be estimated from $P_{SP}$ and $P_{PE}$, as shown in Fig. 6.4,

$$\sigma/e = \frac{[P_{SP}(0) + P_{PE}(x)] - P_{PE}(x)}{e}.$$ (6.8)

When $\Delta P_{SP}$ is greater than $P_{PE}$, the polarisation charges accumulate at the interface of the MgZnO and ZnO layers. On the other hand, when $\Delta P_{SP} < P_{PE}$, the charges will accumulate at the surface of the MgZnO layer.

In this work, polarisation comes from a change in the Mg content in the MgZnO layer. Once this MgZnO is grown, this strain is fixed and cannot be modulated. In this case we apply a dynamic strain wave (SAW) to the ZnO heterostructure to investigate the physical properties of the 2DEG.

### 6.2 SAW-driven lattice displacement

We calculate the lattice displacement in a ZnO substrate when a SAW propagates. In a ZnO wurtzite crystal, the piezoelectric matrix, $e$, elastic matrix, $C$, and dielectric matrix, $\varepsilon$, are given below

$$e = \begin{bmatrix} 0 & 0 & 0 & 0 & e_{15} & 0 \\ 0 & 0 & 0 & e_{15} & 0 & 0 \\ e_{31} & e_{31} & e_{33} & 0 & 0 & 0 \end{bmatrix}$$
Section 6.2. SAW-driven lattice displacement

\[
C = \begin{bmatrix}
C_{11} & C_{12} & C_{13} & 0 & 0 & 0 \\
C_{12} & C_{11} & C_{13} & 0 & 0 & 0 \\
C_{13} & C_{13} & C_{33} & 0 & 0 & 0 \\
0 & 0 & 0 & C_{44} & 0 & 0 \\
0 & 0 & 0 & 0 & C_{44} & 0 \\
0 & 0 & 0 & 0 & 0 & C_{66} \\
\end{bmatrix}
\]

\[
\varepsilon = \begin{bmatrix}
\varepsilon_{11} & 0 & 0 \\
0 & \varepsilon_{22} & 0 \\
0 & 0 & \varepsilon_{33} \\
\end{bmatrix}
\]

The elastic and piezoelectric constants of ZnO depend on the crystal structure, such as thin film or bulk.\(^{178,179}\) In this work, the elastic, piezoelectric and dielectric constants are taken from Ref. 178 (see Table 6.1). Here \(C_{66}\) is equal to \((C_{11} - C_{12})/2\), and \(\varepsilon_{11} = \varepsilon_{22}\). In a ZnO substrate, the stress, \(T\), and the charge displacement, \(D\), are given by:

\[
T = C \cdot S - e^T \cdot E,
\]

\[
D = e \cdot S + \varepsilon \cdot E,
\]

where \(S\) is the strain and \(E\) is the electric field. The displacement and potential functions are then given as

\[
\rho \frac{\partial^2 U}{\partial t^2} = \frac{\partial T_{Xx}}{\partial x} + \frac{\partial T_{Yy}}{\partial y} + \frac{\partial T_{Zz}}{\partial z} + (e_{31} + e_{15}) \frac{\partial^2 \phi}{\partial x \partial z} \tag{6.11}
\]

\[
\rho \frac{\partial^2 V}{\partial t^2} = \frac{\partial T_{Yx}}{\partial x} + \frac{\partial T_{Yy}}{\partial y} + \frac{\partial T_{Yz}}{\partial z} + (e_{31} + e_{15}) \frac{\partial^2 \phi}{\partial y \partial z} \tag{6.12}
\]

\[
\rho \frac{\partial^2 W}{\partial t^2} = \frac{\partial T_{Zx}}{\partial x} + \frac{\partial T_{Zy}}{\partial y} + \frac{\partial T_{Zz}}{\partial z} + e_{31} \frac{\partial^2 \phi}{\partial x^2} + e_{15} \frac{\partial^2 \phi}{\partial y^2} + e_{33} \frac{\partial^2 \phi}{\partial z^2} \tag{6.13}
\]

---

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<th>(C_{12}) (GPa)</th>
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<th>(\varepsilon_{33}) ((\varepsilon_0))</th>
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<td>1.321</td>
<td>-0.44</td>
<td>8.3</td>
<td>9.1</td>
</tr>
</tbody>
</table>

Table 6.1: Elastic, piezoelectric, and dielectric constants in ZnO.\(^{178}\)
\[ \nabla \cdot \mathbf{D} = \frac{\partial D_x}{\partial x} + \frac{\partial D_y}{\partial y} + \frac{\partial D_z}{\partial z} = 0, \]  
(6.14)

where \( U, V \) and \( W \) are the lattice displacement along the \( x \)-axis, \( y \)-axis, \( z \)-axis, and \( \phi \) is potential, and \( \rho \) is the mass density of ZnO. Due to the isotropic properties in the \( xy \)-plane, the calculated \( U \) and \( V \) are the same. The trial solutions for \( U, W \) and \( \phi \) are:

\[ U = U_0 e^{-bkz} e^{ik(x-vt)} \]  
(6.15)

\[ W = W_0 e^{-bkz} e^{ik(x-vt)} \]  
(6.16)

\[ \phi = \phi_0 e^{-bkz} e^{ik(x-vt)}. \]  
(6.17)

To solve these wave equations, we set several boundary conditions. First, \( D \) at the surface is continuous

\[ D_z|_{z=0} (\text{Air}) = D_z|_{z=0} (\text{ZnO}), \]  
(6.18)

which gives

\[ (\varepsilon_{33} - \varepsilon_0) \frac{\partial \phi}{\partial z} = \varepsilon_{31} \left( \frac{\partial U}{\partial x} + \frac{\partial V}{\partial y} \right) + C_{33} \frac{\partial W}{\partial z}. \]  
(6.19)

Then other boundaries are defined at the surface where the stress along the \( z \)-axis is zero

\[ T_{zz} = C_{13} \frac{\partial U}{\partial x} + C_{33} \frac{\partial W}{\partial z} - \varepsilon_{33} \frac{\partial \phi}{\partial z} = 0 \]  
(6.20)

\[ T_{xz} = C_{44} \left( \frac{\partial U}{\partial z} + \frac{\partial W}{\partial x} \right) + \varepsilon_{15} \frac{\partial \phi}{\partial x} = 0. \]  
(6.21)

Then \( U, W \) and \( \phi \) from Eqs. 6.15-6.17 are substituted in Eqs. 6.9-6.14, we can get

\[
\begin{bmatrix}
-\rho v^2 - C_{11} + C_{44} b^2 & -ib(C_{13} + C_{44}) & -ib(\varepsilon_{31} + \varepsilon_{15}) \\
-ib(C_{13} + C_{44}) & -\rho v^2 + b^2 C_{33} - C_{44} & -\varepsilon_{15} + \varepsilon_{33} b^2 \\
-ib(\varepsilon_{15} + \varepsilon_{31}) & \varepsilon_{33} b^2 - \varepsilon_{15} & \varepsilon_{11} - \varepsilon_{11} b^2
\end{bmatrix} \begin{bmatrix} U_0 \\ W_0 \\ \phi_0 \end{bmatrix} = 0
\]  
(6.22)

Then \( b \) is solved as a function of \( v \), where \( v \) is the SAW velocity. There are three possible solutions of \( b \) by solving Eqn. 6.22 (\( b_1, b_2, b_3 \)). Each possible solution contributes to the final trial solutions of \( U, W \) and \( \phi \) with amplitudes of \( R_i U_i, R_i W_i, \) and \( R_i \phi_i \), where \( R_i \) is a weight factor and \( i = 1, 2, 3 \) (see Table. 6.2):

\[ U = (R_1 U_1 e^{-b_1 k z} + R_2 U_2 e^{-b_2 k z} + R_3 U_3 e^{-b_3 k z}) e^{ik(x-vt)} \]  
(6.23)

\[ W = (R_1 W_1 e^{-b_1 k z} + R_2 W_2 e^{-b_2 k z} + R_3 W_3 e^{-b_3 k z}) e^{ik(x-vt)} \]  
(6.24)

\[ \phi = (R_1 \phi_1 e^{-b_1 k z} + R_2 \phi_2 e^{-b_2 k z} + R_3 \phi_3 e^{-b_3 k z}) e^{ik(x-vt)}. \]  
(6.25)

Finally according to the boundary conditions Eqs. 6.18-6.21, \( v \) is estimated to be 2520 ms\(^{-1}\) (most possible one in the three solutions of \( v \)). Meanwhile the weight factor \( R_i \) (here we assume \( R_1 = 1 \)), and the amplitude \( U_i (U_1 = 1), W_i, \) and \( \phi_i \) are also determined by the boundary conditions. Figure 6.5 shows the lattice displacement along the \( x \) and \( z \)-axes (\( U, W \)) and \( \phi \) are functions of the growth depth. This clearly shows that a SAW in ZnO is attenuated over the depth of a wavelength.
Section 6.2. SAW-driven lattice displacement

\[
\begin{array}{ccc}
  b_1 & b_2 & b_3 \\
  -4.66 - 1.83i & -13.38 & -4.66 + 1.83i \\
  R_1U_1 & R_2U_2 & R_3U_3 \\
  1 & 8.67 - 19.16i & -0.66 - 0.75i \\
  R_1W_1 & R_2W_2 & R_3W_3 \\
 -12.86 - 5.82i & 0.22 - 1.76i & 1.47 - 1.00i \\
 R_1\phi_1 & R_2\phi_2 & R_3\phi_3 \\
 1.04e11 - 6.17e9i & 2.68e12 + 1.21e12i & 6.46e10 + 8.29e10i \\
\end{array}
\]

Table 6.2: Calculated coefficients in wave functions.

![Graph](image)

Figure 6.5: Displacement in \( x \) and \( z \)-direction \( U, W \) and the potential \( \phi \) as a function of depth in units of SAW wavelength \( \lambda \).

From this calculation, the lattice displacements at the 2DEG are estimated as a function of time for a fixed SAW amplitude. From Eqns. 6.23-6.25, the displacements in SI unit along the \( a \)-axis \( (A_U) \) and \( c \)-axis \( (A_W) \) are estimated from the displacement in arbitrary unit \( U_{\text{amp}} \) and \( W_{\text{amp}} \) for a given SAW potential amplitude, \( A_{\text{SAW}} \),

\[
U' = U_1R_1 + U_2R_2 + U_3R_3 \\
\theta_U = \arctan \left( \frac{\text{Im}(U')}{\text{Re}(U')} \right) \\
U_{\text{amp}} = \frac{\text{Re}(U')}{\cos(\theta_U)} \\
A_U = \frac{U_{\text{amp}}A_{\text{SAW}}}{\phi_{\text{amp}}} \\
A_W = \frac{W_{\text{amp}}A_{\text{SAW}}}{\phi_{\text{amp}}}.
\]

From the measurements in Chapter 4, the SAW amplitude at a MgZnO/ZnO interface is estimated to be around 100 meV. Therefore the amplitude of displacement
along the \(a\)-axis is around 0.007 \(\text{Å}\) and along the \(c\)-axis is around 0.004 \(\text{Å}\). This difference in \(a\) and \(c\)-axes indicates an elliptical movement of the atoms when a SAW propagates.

### 6.3 SAW-modulated polarisation

![Figure 6.6: Change of lattice constants \(a\) and \(c\) (a) and the strain \(\Delta a/a\) and \(\Delta c/c\) (b) as a function of the SAW phase. The default values of \(a\) and \(c\) for the \(\text{Mg}_{0.1}\text{Zn}_{0.9}\text{O}\) are 3.25 \(\text{Å}\) and 5.193 \(\text{Å}\), and for \(\text{ZnO}\) the values are 3.25 \(\text{Å}\) and 5.2 \(\text{Å}\). (c) Spontaneous polarisation mismatch, \(\Delta P_{\text{SP}}\), and piezoelectric polarisation, \(P_{\text{PE}}\), as a function of SAW phase and (d) the dynamic sheet density \(n_{2\text{D}}\) as a function of the SAW phase. The average effect \(\langle n_{2\text{D}}\rangle\) is indicated as the red dashed line in (d). (c) and (d) are the calculations with a fixed \(\Delta P_{\text{SP}}\), and (e) and (f) are the same calculations but with a SAW-modulated \(\Delta P_{\text{SP}}\) using the point-charge model. Here the SAW amplitude is fixed at 100 meV.

Instead of calculating the 2DEG density as a function of Mg content, we convert it to a function of lattice constants \(a\) and \(c\), and then to a function of SAW propagation phase or time. Because the change in \(a\) and \(c\) is a dynamic process, the strain at the interface is one too. Figure 6.6(a) shows the change in \(a\) and \(c\) as a function of the SAW phase with references to \(a\) (3.25 \(\text{Å}\)) and \(c\) (5.193 \(\text{Å}\)) for \(\text{Mg}_{0.1}\text{Zn}_{0.9}\text{O}\) at a fixed SAW amplitude of 100 mV. The default \(a\) and \(c\) in \(\text{ZnO}\) are 3.25 \(\text{Å}\) and 5.2 \(\text{Å}\), and the strain \(\Delta a/a\) and \(\Delta c/c\) are plotted in Fig. 6.6(b). The sheet carrier density
at the MgZnO/ZnO interface is then calculated as a function of the SAW phase from $\Delta P_{SP}$ and $P_{PE}$, according to Eqns. 6.3, 6.5, 6.8. First, we assume that SAWs modulate both the MgZnO and ZnO layer, and hence that $\Delta P_{SP}$ is independent of SAWs and only dependent on the Mg content. In this case, SAWs only modulate the piezoelectric polarisation, which is calculated using Eqn. 6.3. Figs. 6.6(c) and (d) show $\Delta P_{SP}$, $P_{PE}$, and $n_{2D}$ as a function of the SAW phase. In electron transport measurements, it is difficult to measure this dynamic process at 3 GHz. However, if dynamic changes in $a$ and $c$ have a non-linear effect in the 2DEG density, we may measure the average SAW-modulated 2DEG density, $\langle n_{2D} \rangle$.

![Figure 6.7](image)

**Figure 6.7**: Average sheet density $\langle n_{2D} \rangle$ as a function of SAW amplitude from 0 to 100 meV at different Mg contents $x = 0.05, 0.1, 0.2, 0.3$ with a single SAW beam [(a) and (c)] and two constructively interfering SAW beams [(b) and (d)]. The calculation excluded ((a) and (b)) or included ((c) and (d)) the SAW-modulated $\Delta P_{SP}$.

The polarisation-induced sheet charges accumulate at the interface when $P_{PE} < \Delta P_{SP}$. If instead $P_{PE} > \Delta P_{SP}$, the charge carriers will accumulate at the surface instead of the interface. Without a SAW, it is impossible to reach this regime in a MgZnO/ZnO heterostructure that already has a 2DEG at the interface. However, it is possible to reach this regime at some particular parts of the SAW. However, in experiments, the charges either at the surface or the interface are measured by the same Ohmic contacts. Therefore we can measure both types of charges, and we cannot distinguish the difference between these two regimes in the experiment.

In real experiments, the spontaneous polarisation may also change with SAWs due to the different properties of the MgZnO and ZnO. However, this SAW-
modulated spontaneous polarisation has not been investigated yet. Here we simply use the point-charge model and Eqn. 6.5 with SAW-modulated \( a \) and \( c \). Figures 6.6 (e) and (f) demonstrate the same calculation as in Figs. 6.6 (c) and (d) but include the SAW-modulated \( \Delta P_{SP} \).

Figure 6.7 (a) also shows \( \langle n_{2D} \rangle \) as a function of SAW amplitude in units of meV with different Mg contents in MgZnO from 0.05 to 0.3. We find an increase in \( \langle n_{2D} \rangle \) as the SAW power increases from 0 to 100 meV. When the Mg content is 0.05, the \( \langle n_{2D} \rangle \) first increases and then begins to decrease, and this is because the SAW is strong enough to take the system to the regime \( P_{PE} > \Delta P_{SP} \). Furthermore, if two SAW beams are launched in opposite directions and interfere constructively at the centre of the device, the displacement in the \( a \)-axis is cancelled, and the displacement in the \( c \)-axis is superimposed, forming standing waves. Figures 6.7(b) and (d) give the calculated \( \langle n_{2D} \rangle \) with standing waves or one that only takes account of the strain in the \( c \)-axis. \( \langle n_{2D} \rangle \) also increases with the SAW amplitude, but much more weakly than for a propagating wave. When the Mg content is very high, \( x = 0.3 \), the sheet conductance is almost independent of the SAW amplitude until the amplitude becomes high enough.

Figure 6.8: Schematic diagrams of device Zn-SAW-1 with SAW channels (a) and device Zn-SAW-2 with a small Hall bar (b).

### 6.4 Results and discussions

To investigate the SAW modulation experimentally, we fabricate SAW-devices in MgZnO/ZnO heterostructures. Here we discuss two types of device, as shown in Figs. 6.8 (a) and (b). Device Zn-SAW-1, which uses wafer Zn5-1, contains a pair of split gates with a length of 1.5 \( \mu m \) and a width of 0.7 \( \mu m \), which is similar to that of standard SAW devices in GaAs. The other device Zn-SAW-2 is fabricated on the wafer Zn1-2. There is a small Hall bar, most of which is in the SAW beam.

#### 6.4.1 SAW characterisation

Firstly we characterise SAW generation and propagation using a two-port network analyser, as shown in Fig. 6.9(a). At room temperature, there is no resonance peak
at 2.6 GHz visible above in a high background signal (−40 dB). At this temperature, the non-zero electrical conductivity in a ZnO substrate will screen SAWs, and strongly damp their propagation. As it cools down in a helium dewar, the background signal decreases from −40 dB down to −80 dB, indicating the ZnO substrate becomes better insulating than at room temperature. Hence the SAW resonance peak begins to appear at 2.6 GHz. When the chip is directly above the level of liquid helium, which corresponds to a temperature of 4.2 K, a strong resonance peak appears at around 2.6 GHz, with a peak up to −50 dB. When the chip is dipped into liquid helium, the main resonance peak disappears because of the mass-loading effect, which also proves that the resonance peak is caused by SAWs on the ZnO substrate. The period of the IDT is 1 µm and the SAW speed of this ZnO substrate is around 2600 m s⁻¹, matching the calculation from Eqns. 6.11-6.21. This SAW...
resonance fits a sinc function, as shown in Fig. 6.9(b):

\[
S_{12} = \begin{cases} 
    A \cdot \text{sinc}(N(f - f_0)/f_0) & \text{Without crosstalk} \\
    A \cdot \text{sinc}(N(f - f_0)/f_0) \cdot B \cdot \sin(2\pi f/f_c) & \text{With crosstalk}
\end{cases} \tag{6.31}
\]

where \(A\) is the SAW amplitude, \(B\) is the crosstalk amplitude, \(N\) is the number of pairs of fingers, 70 in our devices, \(f_0\) is the SAW resonant frequency, which is around 2.6 GHz, and \(f_c\) is the crosstalk resonance period, which is around 3 MHz. Compared to the same SAW (\(\lambda = 1 \mu m\)), the bandwidth of the resonant peak on the ZnO substrate is wider than that on a GaAs substrate, and the asymmetry in the main resonant peak is weaker than that in GaAs (see Fig. 3.6(c)). Figure 6.9 (b) also shows the crosstalk between SAWs and electromagnetic waves with an oscillation period of \(\sim 3\) MHz.

### 6.4.2 SAW-modulation in a ZnO 2DEG

![Figure 6.10: Source-drain current \(I_{DC}\) as a function of frequency from 2.4-2.8 GHz at different DC biases at \(V_{SG} = 0\) (a) and \(V_{SG} = -12\) V (b). The RF power is turned on at 2.5 GHz and off at 2.7 GHz.](image)

In device Zn-SAW-1, we apply a small DC bias to one of the Ohmic contacts, with the other one grounded. The source-drain current through a current-voltage pre-amplifier (Model SR570) is measured with a multimeter (Keithley 6514). At \(T = 4\) K, we apply an RF signal to an IDT to observe the SAW-modulation effect. Figure 6.10(a) shows the frequency-dependent current at different DC biases from \(-4.5\) mV to 4 mV. We observe a clear SAW resonance at 2.6 GHz, matching the SAW resonant frequency. When we change the DC bias from \(-4.5\) mV to 4 mV, the SAW resonance stays the same with a dip in the background signal. The resistance of a 2DEG in a MgZnO/ZnO heterostructure is strongly temperature-dependent. The strong RF power will heat the chip. To exclude this heating effect, we turn on the RF power at 2.5 GHz and observe the sudden decrease in the current, which indicates an increase in 2DEG resistance. At 2.7 GHz, we switch off the RF power and observe a sudden increase in current, which indicates a decrease in 2DEG resistance. This is because when the RF signal is turned on, it heats the chip and increases the
Section 6.4. Results and discussions

resistance, and when it is turned off, the chip cools down and the 2DEG resistance decreases. At a positive DC bias, the SAW resonance shows the opposite effect to the heating: the resistance decreases at the SAW resonance frequency. This shows that the dip in resonance is not because of heating. The SAW resonance peak in 2DEG is independent of the source-drain direction and dependent on the SAW propagation direction. This SAW resonance peak cannot be simply explained by the SAW-modulated polarisation, as discussed above.

![Graph](image)

Figure 6.11: (a) Pinch-off characterisation of a SAW channel in a typical GaAs device with and without SAWs. (b) Source-drain current $I_{DC}$ as a function of $V_{SG}$ on (black and blue lines) and off (red line) the resonant frequency for the ZnO device. The arrow indicates SAW-pumping at the gate definition point, which depends on the S-D current direction. The SAW power is 12 dBm.

In a GaAs SAW device, we can achieve the SAW-pumping across a SAW channel. When we sweep the split-gate voltage negatively, electrons below the gates are depleted first, and then electrons between the gates begin to deplete, defining a SAW channel. When SAWs reach the entrance of this SAW channel, SAWs can trap electrons in SAW minima and drag them along the SAW propagation direction. Hence dips or peaks appear at the gate definition voltage or near the SAW channel pinch-off voltage, as shown in Fig. 6.11(a). The dip or peak depends on the SAW propagation direction and the source-drain current direction. Figure 6.11(b) shows the current $I_{DC}$ as a function of $V_{SG}$ with an RF signal on (2.6 GHz) and off.
(2.4 GHz) the SAW resonance. First at gate definition $V_{SG} = -12$ V, we observe an enhancement with a small peak in the current when source-drain electron transport occurs in the same direction that the SAW is travelling in. We then swap the two Ohmic contacts, so that the source-drain electron transport is in the opposite direction to that of the SAW, and the small peak becomes a small dip, which matches the classic SAW-pumping effect. However, the current is still much lower than that of the SAW off-resonance, as shown in Fig. 6.10(b). No matter what is the direction of the SAW and source-drain electron transport, there is a significant drop in the current at all times, even at $V_{SG} = 0$. This effect is different from the usual SAW-pumping in a GaAs SAW device.

Unfortunately, we cannot pinch off the SAW channel in device Zn-SAW-1. When we sweep $V_{SG}$ to more negative value, large electric fields from the gates cause serious leakage through the insulator to the 2DEG. Therefore the well-known quantised SAW-pumping cannot be investigated in this MgZnO/ZnO heterostructure.

This anomalous SAW-modulation cannot be simply explained by either the classic SAW-pumping or the SAW-modulated charge polarisation. In calculations, we assume a fixed SAW amplitude. However, in a real device, the SAW amplitude is attenuated because of the electric screening effect of the 2DEG. Therefore when a SAW passes through the mesa over tens of micrometres, the SAW is attenuated and so the SAW amplitude decreases. As shown in Fig. 6.7, the 2DEG density should increase as the SAW amplitude increases. However, because of the SAW screening effect, the decreasing SAW amplitude results in a decreasing $n_{2D}$ along the mesa, which is equivalent to applying a small DC bias along the direction of the SAW. In Figs. 6.10 (a) and (b), the SAW resonance becomes smaller as the DC bias changes from negative to positive. This decreasing SAW modulation in the 2DEG applies another negative DC bias, $V_{SAW}$, to the applied DC bias $V_{DC} = V_{app} + V_{SAW}$.

In a $^4$He cryostat at a temperature of 1.2 K, we measured device Zn-SAW-2 with 4 µm SAWs, corresponding to a SAW resonant frequency of 0.66 GHz. To remove the series resistance, we performed four-terminal measurements to investigate the effect of the SAW on the 2DEG resistance, $R_{xx}$. Figure 6.12 shows the frequency-dependent $R_{xx}$ at different SAW powers. At a low SAW power of 0 dBm, we see other resonant peaks in SAW off the resonant frequency, which may result from a resonance of in the cables or other cavities in the measurement system. As the RF power increases, the resonance peak starts to increase, and at a high power of 14 dBm the SAW resonance peak dominates, the peak corresponds to an increase in the 2DEG resistance at the SAW resonance. Meanwhile, as the RF power increases, the heating effect also raises the background noise in $R_{xx}$.

We apply an out-of-plane magnetic field and repeat the measurements, as shown in Fig. 6.13. As the magnetic field increases, the background noise is heavily suppressed, and the SAW resonance peak becomes much clearer. In a strong magnetic field, electrons are in cyclotron motion, making it more difficult for them to become excited by electromagnetic waves. In a GaAs SAW device, the SAW pumping current increases significantly as the out-of-plane magnetic field increases. However, in this ZnO SAW device, the SAW resonance peak is almost constant as the out-of-plane magnetic field increases. This effect indicates this SAW resonance is not the result of the SAW-pumping.
As expected theoretically, a SAW modulates the strain, and therefore the 2DEG density in a MgZnO/ZnO heterostructure. Usually, we measure $n_{2D}$ from the Shubnikov–de-Haas oscillation in $R_{xx}$. However, the heating effect is the main problem in this measurement. Because the Shubnikov–de-Haas oscillations are strongly temperature-sensitive, when a SAW is applied, the electron temperature increases and the Shubnikov–de-Haas oscillations are highly damped, as shown in Fig. 6.14. Alternatively, the SAW can be pulsed with a large on/off ratio, such as 1/10, to minimise the heating. However, this will average the conductance without a SAW and with that when the SAW is on, blurring out any effect in $\langle n_{2D} \rangle$. 

Figure 6.12: 2DEG resistance $R_{xx}$ as a function of RF frequency from 0.5 GHz to 0.8 GHz at different RF powers from 0 dBm to 14 dBm in an increment of 2 dBm.

Figure 6.13: 2DEG resistance $R_{xx}$ as a function of frequency from 0.5 GHz to 0.8 GHz at different magnetic fields from 0 to 4 T at an RF power of 10 dBm. Each spectrum is shifted for clarity.
6.5 Conclusion and further works

Using the same effects that gives rise to the 2DEG in a MgZnO/ZnO heterostructure, we have calculated the SAW-modulated spontaneous and piezoelectric polarisation, as well as the 2DEG density. However, measurements in both device Zn-SAW-1 and device Zn-SAW-2 show a change in the current at the SAW resonance, which depends on the SAW propagating direction and the source-drain current direction. This cannot be fully explained by the calculated SAW-modulated polarisation.

For future investigations, it would be necessary to perform a time-resolved measurement to observe the dynamic modulation in $n_{2D}$ in a MgZnO/ZnO heterostructure. Usually, it is only possible to make a time-resolved measurement in an optical measurement, not the electron transport. As we introduced before, a 2DEG could screen the SAW and decrease the SAW modulation. To minimise SAW attenuation over the mesa, we propose a mesa with a width matching the SAW wavelength. In this case, only one SAW period covers the 2DEG. Then the mesa is connected to a $pn$ junction. By applying a forward bias, we can measure the photon emitted from the $pn$ junction. Then a SAW is launched from an IDT and the time-resolved photon intensity is measured. If the 2DEG is modulated by the SAW, we expect to see oscillations in the photon intensity matching the SAW period. Different to the SdH measurements, heating is not a severe problem in this measurement as long as the RF power is fixed.

In a MgZnO/ZnO heterostructure, the 2DEG density is controlled by the Mg content. There is a minimum requirement for the Mg content to induce enough strain for a 2DEG. We could grow a new MgZnO/ZnO heterostructure and control the Mg content just below the minimum requirement for inducing the 2DEG. On this heterostructure, we could fabricate a device with a small Hall bar matching the SAW wavelength and measure at low temperatures. In normal transport measurement, there is no conductance in the Hall bar. If when a SAW passing through the mesa, conductance can be turned on, and also turned off by switching off the SAW, we can conclude that a SAW can modulate the polarisation and induce a
2DEG at the interface, matching the simulation. Then we can perform quantum Hall measurement to determine the 2DEG density as a function of SAW amplitude. This SAW modulation strain offers a unique method to manipulate the strain in a MgZnO/ZnO heterostructure after growth. This technique can also be applied to a GaN/AlGaN heterostructure to manipulate the piezoelectric polarisation.
Conclusions and future works

7.1 Conclusion

In this thesis, we have introduced three types of semiconductor heterostructures: GaAs/AlGaAs, ZnO/GaAs, and MgZnO/ZnO, and investigated low-dimensional electron transport in them using a surface acoustic wave. GaAs/AlGaAs heterostructures have been widely used in research into mesoscopic physics. With surface metallic gates and electric-field effect, we can create quantum wires or quantum dots in a 2DEG. Here it is essential to calculate the electrostatic potential for different gate designs and voltages. We have optimised boundary conditions for the 3D Poisson equation and implemented proper experimental verifications. In an ungated or exposed surface, we have compared different boundary conditions: Dirichlet, Neumann, and Neumann with a dielectric layer, and found that the calculation with Neumann boundary conditions with a dielectric layer matches the experimental result. When the air dielectric layer is replaced by ZnO, our simulation gave a 0.2 V shift in the pinch-off voltage of a split-gate defined 1D channel, which is also observed in our experiments. Below the active larger of each device, we have also found that it is important to push the boundary condition much deeper than the MBE regrowth interface, which up to now has usually been set as equipotential.

With these calculated electrostatic potential and a transmission model, we have simulated SAW-driven quantised charge transport in an induced lateral $n-i-n$ junction, which has been experimentally observed. Moreover, we also simulated an induced lateral $n-i-p$ junction and verified the possibility of controlling the recombination and generation of a high-repetition single-photon source. In experiments carried out by our colleagues, this photon anti-bunching is observed. However, the quantised SAW charge transport fails to appear, which we have shown is probably because of the weak transverse confinement in the dynamic quantum dot.

SAW-driven quantised charge transport is one of the most famous phenomena in SAW nanoelectronics. However, the quantised plateaus are not accurate for metrological applications, even through several techniques have been tried to improve the quantisation. In another type of gate-defined charge pump, the quantisation is greatly improved by applying a strong out-of-plane magnetic field. However, in a SAW charge pump, the quantisation is highly degraded even at 0.5 T. We have explained and modelled this degradation by the suppression of back-tunnelling and also non-adiabatic corrections in the dynamic quantum dot. Moreover, we have de-
signed a spectroscopy device to probe the energy in such a dynamic quantum dot. The energy difference between the first and second electron in SAW-driven dynamic quantum dot is only around 3 meV, which can also explain why the quantisation is not ideal in such a device. To improve SAW quantisation further, an enhancement in the quantum-dot charging energy is vital.

GaAs is not a good piezoelectric substrate for SAW devices. To improve SAW amplitude, we deposit a ZnO thin film on a GaAs heterostructure using HiTUS. In the sputtering process, the damage to the 2DEG conductance is a severe problem. We have developed a thin Al₂O₃ buffer layer and succeeded in protecting the 2DEG during sputtering. With a ZnO layer, we observed strong SAW enhancement in both scattering parameters and SAW-pumping experiments. With help of the ZnO, the required SAW power for quantisation is greatly reduced, which minimises heating in low-temperature measurements. However, the accuracy of SAW quantisation is not significantly improved with a ZnO layer. This fact indicates that the weak SAW amplitude in the GaAs substrate may not be the main limitation for the SAW quantisation. To confirm this conclusion above, stronger dot confinement is needed.

We then turn to MgZnO/ZnO heterostructures, where the spontaneous and piezoelectric polarisation mismatch induces a 2DEG at the interface. After several years’ development, the mobility and density of 2DEG can compete with a traditional GaAs/AlGaAs heterostructure. We have created quantum wires in such a heterostructure using quantum point contacts and a parylene-C insulator. In these wires, we observed quantised conductance in units of $2e^2/h$ up to $16e^2/h$. From the DC bias spectroscopy and in-plane magnetic field measurements, we estimated the $g$-factor to be around 6.8, which is three times larger than that in a 2DEG or bulk. More interestingly, from the energy spacing in out-of-plane magnetic fields, we have measured the electron effective mass and find that it increases as the 1D subband index increases, which can be explained by strong electron-electron interaction. Because of this strong electron-electron interaction, we observe features similarly the 0.7 anomaly up to the fifth 1D subband, which is almost impossible to observe in a GaAs quantum wire.

A SAW is a combination of a strain wave and a potential wave. The 2DEG in a MgZnO/ZnO heterostructure is very sensitive to piezoelectric polarisation, or to strain. By solving wave equations, we have calculated the SAW-driven elliptical displacement in the lattice constants $a$ and $c$, and the change in spontaneous and piezoelectric polarisation. To measure the SAW-modulation effect experimentally, we designed and fabricated SAW devices in MgZnO/ZnO heterostructures. The strong SAW resonance behaves differently to the classical SAW pumping in a GaAs-based 2DEG. However, this result cannot be explained by the calculation, which expects an increase in the 2DEG density as the SAW amplitude increases. Further time-resolved measurements are necessary to confirm the SAW modulation.

7.2 Future works

7.2.1 GaAs

We have optimised boundary conditions for gate-patterned quantum devices and found the simulation result matches the experimental result very well. When the
gate design becomes much more complicated than a pair of split gates, fringing fields or cross-capacitance become non-negligible in the calculation of electrostatic potential. For example, in quantum devices with complicated gate patterns (as shown in Fig. 7.1), we observe coherent electron tunnelling in SAW-driven dynamic quantum dots. To calculate the electron tunnelling probability through the tunnelling barrier, we need to calculate the electrostatic potential accurately with gate voltages matching experimental values. With optimised boundary conditions, we have succeeded in simulating the electrostatic potential of such a quantum device. In the future, this model will be very useful for simulating more complicated quantum devices in a Si-doped GaAs/AlGaAs heterostructure.

![Figure 7.1: An example of the simulation of a complicated gate-patterned SAW quantum device in Ref. 102.](image)

Because of the absence of intentional dopants, the induced 2DEG shows less scattering and a longer mean free path than a Si-doped 2DEG and the ability to have electrons and holes in one device. Therefore the induced 2DEG or 2DHG will be popular in the future. As has been mentioned earlier, induced quantum devices have stricter requirements on boundary conditions than it in doped devices, and this simulation capability will be useful in the design and analysis of such devices.

In GaAs-based SAW devices, we have made several attempts to improve the quantisation of SAW-pumping and found no significant improvement in plateau accuracy. In the spectroscopy measurement, we find that a relatively small charging energy in a SAW-driven dynamic quantum dot is the biggest limitation. We can improve either transverse or longitudinal confinement to reduce the dimensions of the quantum dot. The longitudinal confinement provided by the SAW can be improved either by enhancing the SAW amplitude or shortening the SAW wavelength. How-
ever, in experiments, we have improved the SAW amplitude with a ZnO layer and
do not observe a significant enhancement of SAW quantisation. Reducing the SAW
wavelength by increasing the SAW frequency may cause severe electromagnetic wave
crosstalk, as well as non-adiabatic errors. For the transverse confinement, we can
narrow the gap between split gates to increase transverse confinement. However,
the weak longitudinal confinement, we think, may still be the main reason for the
weak quantisation.

Motivated by the gate-defined charge pump,\textsuperscript{90,93} we can design an exit gate to
provide extra longitudinal confinement, as seen in Fig. 3.16. With the exit gate,
we change the electron selection process from the back-tunnelling to the forward-
tunnelling. We may improve the quantisation by applying an out-of-plane magnetic
field.\textsuperscript{90} Even then, SAW-driven quantised charge transport may not be a good can-
didate for metrological applications to redefine the ampere. However, the SAW tech-
nique shows great potential and unique properties in long-distance single-electron
transport, which can be used in the future quantum information processes, such as
the qubit transfer between two distant quantum dots.

\subsection{ZnO}
We have observed strong $N.7$ structures in a ZnO quantum wire and explain this
phenomenon as being a consequence of strong electron-electron interaction, which
also matches the theoretical expectation in Bauer’s model.\textsuperscript{161} Moreover, we observe
other complex features in the magnetic-field measurement, as shown in Fig. 5.30.
In the future, it would be useful to collaborate with theorists to build a model to
explain these anomalies. In these ZnO quantum wires, one can also investigate more
interesting 1D physics using strong-correlated electrons. A Tomonaga-Luttinger
liquid is a theoretical model for the interacting electrons in quantum wires where the
Fermi liquid description breaks down.\textsuperscript{180} The spin and charge have different group
velocities and can be separated in Luttinger liquid.\textsuperscript{181,182} A ZnO quantum wire and
strong-correlated electrons may be a very promising candidate to investigate 1D
physics in the Tomonaga-Luttinger liquid (seen usually in long wires), which may
also relate to $N.7$ analogues (seen in the short wire).\textsuperscript{183}

Gate-defined quantum dots have provided a promising approach to realise quan-
tum computing.\textsuperscript{62,184} Electron spin can be initialised, controlled and read-out in
GaAs quantum dots using either optical\textsuperscript{185} or electrical techniques.\textsuperscript{186,187} However,
the spin dephasing time, $T_2^*$, is only around 10 ns, which is limited by the hyperfine
interaction with host nuclear spin in Ga and As.\textsuperscript{188} This limitation is inevitable in a
GaAs device. One method for eliminating nuclear spin decoherence is to use a group-
IV semiconductor, such as silicon or germanium. In a Si/SiGe heterostructure, there
is a long nuclei-induced dephasing time of 360 ns for a double quantum dot, which is
around two orders of magnitude over the GaAs-based double quantum dot.\textsuperscript{189} However,
there are some limitations to Si/SiGe heterostructures. First, high dislocation
density limits the electron mobility in Si/SiGe, which is much lower than in a GaAs
system. The two-fold valley degeneracy may also result in exchange coupling inside
the quantum dot.\textsuperscript{62} Furthermore, charged ionised impurities, such as phosphorus in
Si and Si in GaAs, can couple to the qubit and result in decoherence.\textsuperscript{190}

A quantum-dot quantum computer is still being developed, and it is essential to
discover other host materials beyond GaAs and Si systems. In nature there is only 4\% $^{67}$Zn in Zn isotopes, possessing a 5/2 nuclear spin, and the rest have no nuclear spin. This advantage also gives a long spin coherence time in ZnO, and makes it good alternative for qubits. As well as the nuclear spin, the Rashba spin-orbit interaction is also a source of spin dephasing.\textsuperscript{191} A MgZnO/ZnO heterostructure shows a weak Rashba spin-orbit interaction, which is the second smallest in semiconductor heterostructures.\textsuperscript{130} Furthermore, the electron mobility of 2DEG in a MgZnO/ZnO heterostructure can reach over $1 \times 10^6 \text{cm}^2/\text{Vs}$,\textsuperscript{119} which makes it a competitor to the GaAs/AlGaAs heterostructure and better than the Si/SiGe heterostructure. Moreover, ZnO is a direct band-gap semiconductor with a single parabolic band at the $\Gamma$ point. In a MgZnO/ZnO heterostructure, there are no intentional ionised dopants, which reduces the scattering and is beneficial for the quantum information processing. We have successfully created quantum wires using quantum point contacts. In the future, we propose creating quantum dots to investigate Coulomb blockade, and then double quantum dots for electron spin manipulation and quantum computing.

ZnO is also an excellent piezoelectric material and suitable for SAW applications. With these advantages, it should be possible to achieve high-efficient single-electron spin transfer in distant quantum dots in ZnO, as has been done in GaAs.\textsuperscript{47}
A split-gate device in a Si-doped GaAs heterostructure

$\text{surface} = 2.1852 \times 10^{19}$ # Surface charge density in cm$^{-3}$
$\text{back} = 5.45 \times 10^{17}$ # Back charge density in cm$^{-3}$
$\text{doping} = 0.6 \times 10^{18}$ # Si dopant density in cm$^{-3}$
$\text{V}_{\text{sg}} = -1.1$ # Split-gate voltage in V

```
global{
  simulate3D{}
  # 3D simulation
  # database = "../Syntax/zincblende.in" # Material database
  crystal zb{
    x$_{\text{hkl}}$ = [1, 0, 0]
    y$_{\text{hkl}}$ = [0, 1, 0]
  } # Crystal direction
  substrate{
    name = "GaAs"
  } # GaAs substrate
  temperature = 1 # Simulation temperature 1 Kelvin
}
```

```
grid{
  xgrid{
    line{ pos = 0.0 spacing = 40.0 }
    line{ pos = 3000.0 spacing = 40.0 }
  }
  ygrid{
    line{ pos = 0.0 spacing = 40 }
    line{ pos = 500.0 spacing = 40 }
    line{ pos = 1500.0 spacing = 40 }
    line{ pos = 2000.0 spacing = 40 }
  }
  zgrid{
    line{ pos = -1000 spacing = 50 }
  }
```
line{ pos = -10 spacing = 0.5 }  # Fine mesh size at device surface
line{ pos = 0 spacing = 0.1 }
line{ pos = 1 spacing = 0.1 }
line{ pos = 10 spacing = 1 }
line{ pos = 10 spacing = 1 }
line{ pos = 45 spacing = 5 }
line{ pos = 55 spacing = 5 }
line{ pos = 90 spacing = 0.1 }  # Fine mesh size at 2DEG
line{ pos = 100 spacing = 0.2 }
line{ pos = 110 spacing = 1 }
line{ pos = 120 spacing = 10 }
line{ pos = 400 spacing = 20 }
line{ pos = 1000 spacing = 10 }
line{ pos = 1090 spacing = 0.5 }  # Fine mesh size at MBE regrowth
line{ pos = 1090 spacing = 0.5 }
line{ pos = 1150 spacing = 50 }
line{ pos = 1200 spacing = 100 }
line{ pos = 3100 spacing = 100 }
}
periodic{
x = no
y = no
z = no
}
} <<>
structure{
output_region_index{boxes = no}
output_material_index{boxes = no}
output_alloy_composition{boxes = no}
region{
everywhere{
}
binary{
    name = “GaAs”
}
}
region{
cuboid{
x = [0E0, 3000E0]
y = [0E0, 2000E0]
z = [-1000E0, -990E0]
}
contact { name = air }
binary{
    name = “GaAs”
}
}
region{
cuboid{
    x = [0E0, 3000E0]
    y = [0E0, 2000E0]
    z = [-990E0, 0E0]
}
contact { name = Fermi }
binary{
    name = “Air”
}

region{
    cuboid{
        x = [0E0, 3000E0]
        y = [0E0, 2000E0]
        z = [0E0, 10E0]
    }
    binary{
        name = “GaAs”
    }
}

region{
    cuboid{
        x = [0E0, 3000E0]
        y = [0E0, 2000E0]
        z = [0E0, 90E0]
    }
    ternary_constant {
        name = “Al(x)Ga(1-x)As”
        alloy_x = 0.32E0
    }
}

region{
    cuboid{
        x = [0E0, 3000E0]
        y = [0E0, 2000E0]
        z = [3090E0, 3100E0]
    }
    contact { name = contact 2}
    binary{
        name = “GaAs”
    }
}
region{
    cuboid{
        x = [1150E0, 1850E0]
        y = [0E0, 650E0]
    }
    # 1 μm air layer above the device
    # We set the device surface at zero
    # 10 nm GaAs cap layer
    # 80 nm AlGaAs layer
    # Al content: Al_{0.32}Ga_{0.68}As
    # Back contact
    # deeper than the MBE regrowth interface
    # Split gate (low) with L=700 nm
    # and W=700 nm
```plaintext
z = [0E0, 2E0] # For GaAs Schottky barrier
}
cuboid{
    x = [1150E0, 1850E0]
y = [1350E0, 2000E0]
z = [0E0, 2E0]
}
contact { name = gate_gaas }
binary{
    name = “GaAs”
}
}
region{
    cuboid{
        x = [1150E0, 1850E0]
y = [0E0, 650E0]
z = [-20E0, 0E0] # For Air Schottky barrier
    }
cuboid{
    x = [1150E0, 1850E0]
y = [1350E0, 2000E0]
z = [-20E0, 0E0]
    }
contact { name = gate_air }
binary{
    name = “GaAs”
}
}
region{
    cuboid{
        x = [0E0, 3000E0]
y = [0E0, 2000E0]
z = [10E0, 50E0]
    }
doping{
        constant{
            name = “impurity”
            conc = $doping # 0.6 \times 10^{18} \text{ cm}^{-3}$
        }
    }
}
region{
    cuboid{
        x = [0E0, 3000E0]
y = [0E0, 2000E0]
z = [0E0, 1E0] # Delta doping
    }
}
```
doping{
  constant{
    name = “surface”
    conc = $surface # 2 \times 10^{19} \text{ cm}^{-3}
  }
}

region{
  cuboid{
    x = [0E0, 3000E0]
    y = [0E0, 2000E0]
    z = [1089E0, 1090E0]
  }
  doping{
    constant{
      name = “back”
      conc = $back # 5.45 \times 10^{17} \text{ cm}^{-3}
    }
  }
}

impurities{
  donor{
    name = “impurity”
    energy = -1000E0
    degeneracy = 2
  }
  acceptor{
    name = “surface”
    energy = -1000E0
    degeneracy = 4
  }
  acceptor{
    name = “back”
    energy = -1000E0
    degeneracy = 4
  }
}

contacts{
  ohmic{
    name = air
    bias = 0.0e0
  }
  schottky{
    name = contact2
    bias = 0.0e0
    barrier = 0.75
  }
}
# From the Fermi level
# to the edge of conduction band.

schottky{
    name = gate_gaas
    bias = $V_{sg}$
    barrier = 0.75
}

schottky{
    name = gate_air
    bias = $V_{sg}$
    barrier = 7.5
}  # Schottky barrier for Air (Half bandgap of Air)

fermi{
    name = Fermi
    bias = 0.0e0
}  # Set the Fermi level

} <<
classical{
    Gamma{}
    HH{}
    LH{}
    output_bandedges{averaged = no }  # Output Band structures
    output_carrier_densities{}
    output_intrinsic_density{}
}

} <<
poisson{
    output_electric_field{}
    output_potential{}
    newton_solver{
        iterations = 50
        search_steps = 40
        residual = 1e-4
    }
}

} <<
currents{
    output_fermi_levels{}
}

} <<
quantum{
    region{
        name = "quantum_region"
        x = [0E0, 3000E0]
        y = [0E0, 2000E0]
        z = [85E0, 100E0]
        boundary{
            x = dirichlet
            y = dirichlet
        }
    }

}  # For Schröedinger solver
# In our model Usually for the 1D simulation, not for 3D

# Z boundary for Schröedinger solver
z = dirichlet
}  Gamma{
    num_ev = 10
}
output_wavefunctions{
    max_num = 10
    all_k_points = yes
    amplitudes = no
    probabilities = yes
}

# Solves for the Gamma conduction band
# Number of eigenvalues

# Output wave function
# Number of eigenfunctions to print out

# User’s define output files in .dat
# Output a 1D section of the simulation area (1D slice)
# Name of section enters file name
# At x = 1500 nm
# At y = 1000 nm

# Output a 1D section of the simulation area (1D slice)
# At x = 1500 nm
# At z = 91 nm

# Output a 1D section of the simulation area (1D slice)
# At y = 1000 nm
# At z = 91 nm

# Output a 2D section of the simulation area (2D slice)
# At z = 91 nm

# Solving Poisson equation
# Solving Schröedinger equation
# Solving Schröedinger, Poisson (and current)
# Self-consistently
<table>
<thead>
<tr>
<th>Abbreviation</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>SAW</td>
<td>Surface acoustic wave</td>
</tr>
<tr>
<td>FET</td>
<td>Field-effect transistor</td>
</tr>
<tr>
<td>3D</td>
<td>Three-dimensional</td>
</tr>
<tr>
<td>2D</td>
<td>Two-dimensional</td>
</tr>
<tr>
<td>1D</td>
<td>One-dimensional</td>
</tr>
<tr>
<td>0D</td>
<td>Zero-dimensional</td>
</tr>
<tr>
<td>2DEG</td>
<td>Two-dimensional electron gas</td>
</tr>
<tr>
<td>2DHG</td>
<td>Two-dimensional hole gas</td>
</tr>
<tr>
<td>DOS</td>
<td>Density of states</td>
</tr>
<tr>
<td>HEMT</td>
<td>High-electron-mobility-transistor</td>
</tr>
<tr>
<td>QD</td>
<td>Quantum dot</td>
</tr>
<tr>
<td>QW</td>
<td>Quantum well</td>
</tr>
<tr>
<td>IDT</td>
<td>Inter-digital transducer</td>
</tr>
<tr>
<td>RF</td>
<td>Radio frequency</td>
</tr>
<tr>
<td>PL</td>
<td>Photo-luminescence</td>
</tr>
<tr>
<td>EL</td>
<td>Electric-luminescence</td>
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<tr>
<td>CAP</td>
<td>Coherent acoustic phonons</td>
</tr>
<tr>
<td>DQD</td>
<td>Dynamic quantum dot</td>
</tr>
<tr>
<td>QED</td>
<td>Circuit quantum electrodynamic</td>
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<tr>
<td>BCs</td>
<td>Boundary conditions</td>
</tr>
<tr>
<td>PDE</td>
<td>Partial differential equation</td>
</tr>
<tr>
<td>FEM</td>
<td>Finite-element method</td>
</tr>
<tr>
<td>MBE</td>
<td>Molecular-beam epitaxy</td>
</tr>
<tr>
<td>HiTUS</td>
<td>High-target-utilisation sputtering</td>
</tr>
<tr>
<td>ALD</td>
<td>Atomic-layer deposition</td>
</tr>
<tr>
<td>PLD</td>
<td>Pulsed layer deposition</td>
</tr>
<tr>
<td>AFM</td>
<td>Atomic force microscope</td>
</tr>
<tr>
<td>Abbreviation</td>
<td>Description</td>
</tr>
<tr>
<td>--------------</td>
<td>-------------</td>
</tr>
<tr>
<td>SEM</td>
<td>Scanning electron microscopy</td>
</tr>
<tr>
<td>XRD</td>
<td>X-ray diffraction</td>
</tr>
<tr>
<td>ESR</td>
<td>Electron spin resonance</td>
</tr>
<tr>
<td>FWHM</td>
<td>Full width of half maximum</td>
</tr>
<tr>
<td>HF</td>
<td>Hydrofluoric</td>
</tr>
<tr>
<td>IPA</td>
<td>Isopropyl alcohol</td>
</tr>
<tr>
<td>PMMA</td>
<td>Polymethyl methacrylate</td>
</tr>
<tr>
<td>CPW</td>
<td>Coplanar-waveguide</td>
</tr>
<tr>
<td>LO</td>
<td>Longitudinal optic</td>
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<tr>
<td>SdH</td>
<td>Shubnikov—de-Haas</td>
</tr>
<tr>
<td>MOSFET</td>
<td>Metal-oxide-semiconductor-field-effect-transistor</td>
</tr>
<tr>
<td>PEDOT: PSS</td>
<td>poly(3,4-ethylenedioxythiophene): poly(styrene-sulfonate)</td>
</tr>
<tr>
<td>QPC</td>
<td>Quantum point contact</td>
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<tr>
<td>CB</td>
<td>Coulomb-blockade</td>
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<tr>
<td>P&lt;sub&gt;SP&lt;/sub&gt;</td>
<td>Spontaneous polarisation</td>
</tr>
<tr>
<td>P&lt;sub&gt;PE&lt;/sub&gt;</td>
<td>Piezoelectric polarisation</td>
</tr>
</tbody>
</table>


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