

Copyright is owned by the Author of the thesis. Permission is given for a copy to be downloaded by an individual for the purpose of research and private study only. The thesis may not be reproduced elsewhere without the permission of the Author.

DIFFERENTIAL CONDUCTANCE OF A BALLISTIC QUANTUM WIRE IN THE PRESENCE OF RASHBA SPIN–ORBIT AND ZEEMAN INTERACTIONS

A thesis presented in partial fulfilment of the requirements

for the degree

of Master of Philosophy

in Theoretical Condensed Matter Physics at Massey University New Zealand

> Nitin Roy Nand 2007

Copyright © 2007 by Nitin Roy Nand

Contents

	Abs	stract	iii			
	List of Figures					
	Acknowledgements					
1	oduction and Background	1				
	1.1	The two-dimensional electron gas	2			
	1.2	Mesoscopic systems and ballistic quantum wires	3			
	1.3	Past work on quantum wires	4			
		1.3.1 Quantum wire with Rashba effect	4			
		1.3.2 Quantum wire with Rashba effect and magnetic fields	5			
	1.4	The purpose of this thesis	6			
2	The	oretical Methodology	7			
	2.1	The quantum wire model	7			
		2.1.1 The Rashba spin–orbit interaction	7			
		2.1.2 The Zeeman interaction	9			
	2.2	The normal and full Rashba regimes	11			
	2.3	Solving an eigenvalue Hamiltonian problem	13			
	2.4	The derivation of the differential conductance formula	14			
3	3 Dispersions					
	3.1	Normal Rashba dispersions	17			
		3.1.1 Transverse (x) magnetic field	17			
		3.1.2 Parallel (y) and perpendicular (z) magnetic field	18			
	3.2	Full Rashba dispersions	20			
		3.2.1 Transverse (x) magnetic field	20			
		3.2.2 Parallel (y) magnetic field \ldots	20			
		3.2.3 Perpendicular (z) magnetic field	23			
4	Diff	erential Conductance	25			
	4.1	Differential conductance results	25			
		4.1.1 Normal Rashba differential conductance	25			
		Set 1: Transverse (x) magnetic field	26			

	4.2	4.1.2 Discuss	Set 2: Parallel (y) and perpendicular (z) magnetic field20Full Rashba differential conductance20Set 1: Transverse (x) magnetic field31Set 2: Parallel (y) magnetic field32Set 3: Perpendicular (z) magnetic field33Sion40	6 6 2 2 0					
5	Sum	mary a	nd Conclusion 4	3					
A	Phy A.1 A.2	sical Ha Norma Full Ra	miltonian expressions4Rashba Hamiltonian expressions4shba Hamiltonian expressions4	5 5 6					
B	Mat B.1 B.2	rix repr Norma Examp	esentations of the Hamiltonians4'and full Rashba Hamiltonian matrix expressions4'les of Hamiltonian matrix expressions and their eigenenergy levels4'	7 7 8					
C	C Typical physical parameters encountered in GaAs/AlGaAs heterostructures and their values								
Bibliography									

Abstract

This thesis calculates the theoretical differential conductance of a ballistic quantum wire semiconductor nanostructure in the presence of Rashba spin–orbit and Zeeman interactions. In semiconductor heterostructures the Rashba spin–orbit interaction arises due to structure inversion asymmetry and couples the spin of the electron to its orbital momentum. In our work Zeeman interaction is induced by application of external magnetic fields in directions transverse, parallel, and perpendicular to the wire axis. Differential conductance is defined as the rate of change of current with respect to a voltage which is applied between two contacts, one on the left (source) and the other on the right (drain) side of the nanostructure.

The dispersion relations of the wire are obtained and from these differential conductance is calculated. Differential conductance is presented for zero and strong spin–orbit interaction situations and for magnetic fields applied in the various directions. The wire is studied under two specific regimes, namely normal and full Rashba mediated by the Rashba spin–orbit Hamiltonian. In the normal Rashba regime the wire is modelled without Rashba intersubband coupling while the full Rashba model includes this coupling.

Spin–orbit interaction and the direction of applied magnetic field significantly modifies dispersions and have drastic effects on the differential conductance profile. The application of magnetic field in directions parallel (and perpendicular) to the wire in the normal regime in the strong Rashba limit results in the formation of energy gaps. The presence of these gaps drastically reduces conductance. These gaps are suppressed in the full Rashba model of the wire in the strong Rashba limit and therefore reduction in conductance is not observed in the parallel and perpendicular field directions. In the normal Rashba regime in the strong Rashba limit conductance is enhanced for a greater range of source–drian bias voltages at low fields, especially for fields applied in the parallel (and perpendicular) directions. Whereas, in the full Rashba regime in the strong Rashba limit conductance is enhanced upto mid range fields and voltages for all field directions. In both Rashba regimes in the strong Rashba limit the overall conductance is reduced at low fields and voltages for all field directions. Hence, it is concluded that weak Zeeman and weak spin–orbit effects at low bias voltages favours electron transmission in ballistic quantum wires.

List of Figures

1.1	Schematic of the two-dimensional electron gas formed at the interface of $n-AIGaAs/i-GaAs/Si-GaAs$ heterojunction by the bending of the conduction (E _C) and valence (E _V) energy bands. The Fermi level is shown by E _F . Adapted from [9].	2
2.1 2.2	Schematic dispersions showing splitting for one subband only. (a) Zero Rashba and Zeeman spin splitting, (b) due to strong Rashba splitting at zero magnetic field, and (c) in the presence of a strong magnetic field only (Zss). The solid and broken curves represent the spin–split states Schematic of the quantum wire studied in this thesis showing the coordinate system and the source (S) and drain (D) contacts	10
	hate system and the source (3) and drain (D) contacts	11
3.1	Dispersions for strong Rss corresponding to (a) zero and (b) maximum magnetic fields applied in the transverse (x) , and (c) for maximum magnetic fields applied in the parallel (u) directions in the normal Rashba wire	
	model.	19
3.2	The evolution of dispersions for strong Rss and magnetic field applied in the transverse (x) direction in the full Rashba wire model	21
3.3	The evolution of dispersions for strong Rss and magnetic field applied in the parallel (y) direction in the full Rashba wire model.	22
3.4	The evolution of dispersions for strong Rss and magnetic field applied in the perpendicular (z) direction in the full Rashba wire model.	24
4.1	Density ΔG plots for transversely applied magnetic field B_x at zero and strong Rss in the normal Rashba wire model	27
4.2	Parametric3D ΔG plots as a function of V_{sd} at fixed transverse magnetic field B_{sd} and as a function of B_{sd} at fixed V_{sd} for zero and strong Rss in the	21
	normal Rashba wire model	28
4.3	2D ΔG plots as a function of V_{sd} at zero transverse magnetic field B_x and as a function of B_x at zero V_{sd} for zero and strong Rss in the normal	
	Rashba wire model	29
4.4	Density ΔG plots for parallelly applied magnetic field B_u for zero and	
	strong Rss in the normal Rashba wire model.	30
4.5	Parametric3D ΔG plots as a function of V_{sd} at fixed parallel magnetic	
	field B_{μ} for zero and strong Rss in the normal Rashba wire model	31

LIST OF FIGURES

4.6	Density ΔG plots for transversely applied magnetic field B_x for zero and	
	strong Rss in the full Rashba wire model.	33
4.7	Parametric3D ΔG plots as a function of V_{sd} at fixed transverse magnetic	
	field B_x for zero and strong Rss in the full Rashba wire model	34
4.8	2D ΔG plots as a function of V_{sd} at zero transverse magnetic field B_x and	
	as a function of B_x at zero V_{sd} for zero and strong Rss in the full Rashba	
	wire model	35
4.9	Density ΔG plots for parallelly applied magnetic field B_y for zero and	
	strong Rss in the full Rashba wire model.	36
4.10	Parametric3D ΔG plots as a function of V_{sd} at fixed parallel magnetic	
	field B_y for zero and strong Rss in the full Rashba wire model	37
4.11	Density ΔG plots for perpendicularly applied magnetic field B_z for zero	
	and strong Rss in the full Rashba wire model.	38
4.12	Parametric3D ΔG plots as a function of V_{sd} at fixed perpendicular mag-	
	netic field B_z for zero and strong Rss in the full Rashba wire model	39
4.13	Schematic dispersions showing how states are filled and emptied with	
	zero and changing source-drain bias voltage and different spin splitting	
	scenarios (closed circles are occupied and open are empty states)	42

v

Acknowledgements

I thank the Institute of Fundamental Sciences (IFS)–Physics, College of Sciences, Massey University, Palmerston North, New Zealand for the opportunity to undertake the Master of Philosophy Degree in Theoretical Condensed Matter Physics. I sincerely thank my supervisor Dr. Ulrich Zülicke for identifying a suitable project for my thesis, his guidance and suggestions, sparing his time for me always, and his enlightening criticisms on the subsequent drafts. A special thank you goes to Dr. François Bissey of IFS–Physics for providing expertise on the LATEX system for the preparation of this thesis. I also take this opportunity to dearly and heartfully thank my Mum and Dad for their moral and financial support, well wishes, and prayers.

Nitin Roy Nand November, 2007.

Chapter 1 Introduction and Background

Over the past two decades the discovery of conductance quantisation in quantum point contacts and two-dimensional electron systems in a quantising magnetic field has initiated extensive research towards investigating transport properties in nanostructures related to the charge of the electron. In addition, the Coulomb blockade in quantum dots connected to conducting leads by high tunner barriers can be used to construct a singleelectron transistor, in which switching between non-conducting and conducting states is done with a single charge [1, 2, 3]. Transport phenomenon in nanostructures that utilise the spin of the electron towards the understanding, designing, and implementation of novel spin-based electronic devices, however, have attracted considerable interest only during the past few years after the theoretical design of a spin-based transistor by Datta and Das in 1990 [4]. The field of spin electronics commonly known as spintronics includes the spin degree of freedom of an electron in addition to its charge and is a rapidly emerging, promising, and intriguing subject. Spintronics aims to bring novel functionalities to conventional electronic devices via the manipulation of electron spin by various means, such as imposing external electrical and magnetic fields to control and manipulate charge and spin dynamics. Although, advances have been made over the years in many areas including spin transport, spin dynamics, and spin relaxation, the full potential of spintronic applications in nanoscale electronic devices are yet to be developed and physically realised [5]. The cornerstone of the many advances in spintronics todate is the two-dimensional electron gas (Section 1.1).

Emerging research in the field of semiconductor nanoelectronics technology and mesoscopic physics have widely focused on the potential use of electron spin [3, 6]. The investigations encompass the broad field of spin-dependent quantum transport. One of which may involve studying ways in which electron spin can be effectively injected, manipulated, controlled, and detected across a semiconductor nanostructure and hybrid magnetic systems. Injecting electrons into a semiconductor from a ferromagnet is a standard way to generate spin-polarised current [7]. The giant magnetoresistance (GMR) effect, which was discovered in magnetic multilayers (consisting of an alternate stack of ferromagnetic and non-ferromagnetic metallic layers) finds applications in devices, such as GMR magnetic sensors and computer hard disk drive read heads for ultra high density magnetic recording [8]. Spin injection, manipulation, control, and detection are important



Figure 1.1: Schematic of the two-dimensional electron gas formed at the interface of n-AlGaAs/i-GaAs/Si-GaAs heterojunction by the bending of the conduction (E_C) and valence (E_V) energy bands. The Fermi level is shown by E_F. Adapted from [9].

considerations even in the design and development of novel futuristic spin-based electronic devices, such as spin-field effect transistors and circuits for spin-based quantum information processing [2].

1.1 The two-dimensional electron gas

The theoretical work reported in this thesis are based on GaAs-AlGaAs heterojunctions where a thin conducting layer is formed at the interface between GaAs and AlGaAs known as the two-dimensional electron gas (or 2deg in short). Since the Fermi energy of the wide gap AlGaAs layer is higher than that in the narrow gap GaAs layer. electrons spill over from AlGaAs (which is n-doped) leaving positively charged donors. This space-charge distribution gives rise to a triangular shaped electrostatic potential that causes the conduction and valence bands to bend as shown in Fig. 1.1. At equilibrium the Fermi energy is constant everywhere [10]. The advantages of using 2degs include mean free paths and coherence lengths that exceed tens of microns at low temperatures. These heterostructures have progressed tremendously since the early 1980s and provide the best realisation of a two-dimensional metal available today with very high electron mobilities corresponding to mean free paths larger than typical device dimensions [10, 11]. In these 2degs the electrons are confined along one direction, typically the perpendicular z axis, which is also the growth direction of the heterostructure, in the lowest quantum mechanical state at the GaAs/AlGaAs interface often referred to as a 2D quantum well. Thus, free-moving electrons with a renormalised effective mass $m = 0.067m_{o}$ (where m_o is the free electron mass) are only present in the remaining two dimensions (in-plane x and y) and are situated typically around 100 nm below the surface. The combination of intrinsic and silicon doped GaAs and n-AlGaAs semiconductor materials which have ideal properties, such as identical lattice constants (which minimises strain) and super clean growth conditions result in nearly defect free interfaces. Moreover, advanced modulation doping techniques removes the ionised Si-donor atoms away from the interface, which minimises scattering allowing the fabrication of extremely high mobility 2degs [10, 11, 12]. The practical importance of the 2deg lies in its use as field–effect transistors and are referred to as modulation doped field–effect (MODFET) or high electron mobility transistors (HEMT). Transistors built on these 2degs have the lowest noise, highest frequency responses, and superior power handling efficiencies and find extensive use in telecommunication applications. These electron gases even display integer [13] and fractional quantum Hall effects [14, 15, 16, 17] if cooled to low temperatures and placed in high magnetic fields.

The two-dimensional electron gas facilitates the study of low-dimensional physics in both theoretical and experimental aspects. The 2deg provides a platform where lowdimensional semiconductor devices can be experimentally realised by further nanostructuring the 2deg. The methods used can range from advanced lithography, molecular beam epitaxy, or ion beam implantation techniques [10, 11, 18, 19] to create mesoscopic devices of reduced dimensions, such as quantum wires, quantum point contacts, and quantum dots. Further limiting the motion of an electron in one or more spatial directions within the 2deg semiconductor heterostructure plane leads to quantum confinement. Quantum confinement gives rise to new and fundamentally important physics phenomenon, which otherwise is diminished in bulk 3D semiconductors and metals. It is therefore interesting to study quantum transport through these quantum confined mesoscopic systems. For a comprehensive review of quantum transport in semiconductor nanostructures and mesoscopic systems the reader is referred to Refs. [20, 21, 22].

1.2 Mesoscopic systems and ballistic quantum wires

Mesoscopic systems are of nanometric size as they lie in-between microscopic and macroscopic systems. Since mesoscopic systems are so small they rely on a completely quantum mechanical approach rather than a classical one to describe its electron transport properties, such as transmission and conductance. The most important parameters (or length scales) that describe mesoscopic systems are the phase coherence length ℓ_{ϕ} , Fermi wavelength λ_F , and the mean free path ℓ_e of electrons. In a mesoscopic device the ℓ_{ϕ} is much larger than the physical dimensions (length L and width W) of the device, while the λ_F is comparable to these dimensions. This means that the electron's wavefunction is coherent and the electron can physically "move" within the device as matter waves giving rise to interference effects. If ℓ_e is much larger than L and W the device is a *ballistic* one in which electrons propagate through the device without being scattered (either elastically or inelastically) due to impurities or phonons [23, 24, 25].

Ballistic quantum wires have been proposed as basic elements in the design of spin filters and spin transistors [26]. It is a central requirement to control and manipulate the spin of electrons with electric fields to realise such spintronic devices. In semiconductor heterostructures (2deg) the macroscopic electric field present along the z direction is a source of intrinsic spin–orbit effects [27, 28, 29, 30, 31]. These spin–orbit effects can

be controlled and manipulated using split gates. Datta and Das [4] were first to describe how the electrical field of an external gate electrode could be used to manipulate the spin precession of a conduction electron. Crucial to this mechanism is the field-dependent spin-orbit interaction, which in narrow gap 2degs is modelled by the Rashba spin-orbit interaction (Rsoi) Hamiltonian (discussed in Chapter 2). The Rashba spin-orbit strength increases linearly with the electron wavevector [32]. Other authors, such as Nitta et al [33] and Grundler [34] have also demonstrated the tuning of the Rashba coupling by an external gate voltage and application of a back gate voltage in different semiconductors, respectively. Matsuyama et al [35] have also established the same in a p-type InAs semiconductor.

1.3 Past work on quantum wires

A vast range of literature is available which investigates various electronic transport properties in quantum wires and quasi-one dimensional electron systems (Q1Des). This thesis is focused on the electron transport properties of ballistic quantum wires with Rashba spin-orbit interactions and application of external magnetic fields. In this Section a few examples of work related to this thesis are presented highlighting the significant results. Studies on quantum wires with Rashba effect only are considered first followed by studies including magnetic fields.

1.3.1 Quantum wire with Rashba effect

Ando and Tamura [36] have investigated conductance fluctuations in quantum wires in the presence of strong Rashba effect but in the absence of a magnetic field. They reported that a strong spin-orbit interaction reduces the fluctuations by half. This result coincides with ours at zero bias voltages for a similar situation. The effect of the spinorbit interaction arising via a lateral confinement potential and also from a perpendicular one (Rashba type) on the band structure and conductance of Q1Des were carried out by Moroz and Barnes [37]. They found that the spin-orbit contributions from these two different spatially directed potentials significantly affect the band structure by introducing a wavevector dependence to subband energies producing additional subband minima and inducing anticrossings between subbands. This observation is reported in this thesis at zero fields and strong Rashba spin-orbit effects as well.

Governale and Zülicke [38] presented analytical and numerical results for strong Rashba spin–orbit coupling on band structure, transport, and interaction effects in quantum wires. They found that for situations with only the lowest spin–split subbands occupied, the electrons close to the Fermi points of the same chirality can have approximately parallel spins. In another study of Rashba spin splitting in quantum wires conducted by Governale and Zülicke [39], they reported hybridisation of spin–split quantum wire subbands in cases of strong Rashba effect. They reported that hybridisation led to unusual spin structures, where the direction of motion of electrons can fix their spin states. This property is claimed to have important ramifications for linear transport in quantum wires giving rise to spin accumulation without magnetic fields or ferromagnetic contacts.

1.3.2 Quantum wire with Rashba effect and magnetic fields

Berggren et al [40] have studied the magnetoconductance of 1D subbands in a narrow 2deg in a GaAs/AlGaAs heterojunction and have reported magnetic field induced depopulation of the 1D subbands in the presence of a transverse magnetic field. A similar depopulation of 1D subbands was reported by Berggren et al [41] in narrow quasi-one dimensional quantum channels, this time by an application of a perpendicular field. In our study subband depopulation due to magnetic fields applied transverse, parallel, and perpendicular to the wire are reported consistently for both zero and strong spin-orbit situations. Zhao et al [42] have also reported magnetic depopulation of an axial magnetic field.

Moroz and Barnes [43] have theoretically studied the effect of spin-orbit interaction on band structure and low temperature transport in long Q1Des in zero and weak magnetic fields applied perpendicular to the nanostructure. They reported that spin-orbit interaction has peculiar effects on the band structure. A study on antisymmetric spin filtering in Q1Des with uniform spin-orbit coupling and presence of a weak in-plane magnetic field was presented by Středa and Šeba [44]. They discovered the presence of an energy interval (a gap) in the electron energy spectrum at which the orientation of spin states is controlled by the direction of the electron velocity leading to the natural spin polarisation of the electron current, if the Fermi energy falls into this energy interval. The effect of spin-orbit interactions (without Rashba intersubband coupling) and in-plane magnetic fields on the conductance of a ballistic Q1Des was studied by Pershin et al [45]. They found that the interplay of the spin-orbit interaction with effective magnetic field significantly modifies the band structure producing additional subband extrema and energy gaps. Hence, introducing the dependence of the subband energies on the field direction. The presence of energy gaps are reported in this thesis for fields applied parallel (inplane) and perpendicular to the wire axis for a similar model of the wire, as will be seen in Chapter 3. Serra et al [26] have analysed the spectral and transport properties of ballistic Q1Des in the presence of spin-orbit coupling and in-plane magnetic fields. Their results demonstrate that Rashba precession and intersubband coupling must be treated on equal footing for wavevectors near the magnetic-field-induced gaps. They found that intersubband coupling limits the occurrence of negative effective masses at the gap edges and modifies the linear conductance curves in the strong-coupling limit. Our study extends the work done by Serra et al [26] and Pershin et al [45] by including perpendicularly applied external magnetic fields and most significantly the application of a source-drain bias voltage to investigate its effect on the transport properties of a ballistic quantum wire.

Pereira and Miranda [46] investigated the effect of strong spin-orbit interaction on electronic transport through non-magnetic impurities in one-dimensional systems. When a perpendicular magnetic field is applied the electron spin polarisation becomes momentum dependent and spin-flip scattering appears to first order in the applied field, in addition to the usual potential scattering. They analysed a situation in which by tuning the Fermi level and the Rashba coupling the magnetic field can suppress the potential scattering. Debald and Kramer [47] investigated the influence of a perpendicular magnetic field on the spectral and spin properties of a ballistic Q1Des with Rashba effect. The magnetic field strongly alters the spin-orbit induced modification to the subband structure when the

magnetic length becomes comparable to the lateral confinement. A subband-dependent energy splitting at k = 0 is found, which can be much larger than the Zeeman splitting attributed to the breaking of a combined spin orbital-parity symmetry. A similar subband energy splitting at k = 0 is also found in our work for perpendicularly applied fields in the absence of Rashba intersubband coupling.

Even though spin-orbit effects and magnetic field dependent electronic transport in quantum wires have been studied quite extensively in the past, a single investigation of the differential conductance of non-interacting electrons with source-drain bias voltage V_{sd} for both in-plane (transverse and parallel) and perpendicular magnetic fields with strong Rashba spin-orbit interaction has been lacking. The purpose of this thesis is to bridge this deficiency in the existing literature and contribute further to the existing knowledge in this field.

1.4 The purpose of this thesis

The process of electron transmission through quasi-one dimensional electron systems involves the redistribution of incoming electron fluxes amongst its discrete eigenenergy levels followed by adiabatic transport through them. The determination of the electron eigenenergies of a Q1Des is an integral part of solving a more general quantum transport problem. This is usually obtained via a numerical diagonalisation of an Hamiltonian that describes the motion of these electrons in the system. As this approach is particularly relevant to the ballistic transport regime [37, 48] similar to that investigated in our work, we use this same approach. Once the eigenenergies are known these are used to produce dispersion relations to deduce the band structure of the Q1Des. By varying a physical parameter, such as the source-drain bias voltage to probe the band structure the differential conductance can be calculated. This is the methodology used in our study to investigate the differential conductance of a ballistic quantum wire. Differential conductance $\triangle G$ is defined as the rate of change of current I with respect to the source-drain voltage V_{sd} (i.e., $\triangle G = dI/dV_{sd}$) and is discussed in Chapter 2.

The objective of this thesis is: i) to theoretically calculate the differential conductance of a ballistic quantum wire from the wire's electronic band structure (dispersion relations) in the presence of Rashba spin–orbit and Zeeman interactions, and ii) to investigate the interplay between the Rashba and Zeeman effects on the wire's differential conductance. This thesis shows how the differential conductance of a ballistic quantum wire varies with source–drain voltage, magnetic fields applied in various directions with respect to the wire axis, and with and without the Rashba spin–orbit interaction.

The organisation of this thesis is as follows: Chapter 2 discusses the theoretical aspects of the quantum wire investigated in this work and lays down the theoretical methodology; Chapter 3 presents the dispersions for the wire and discusses the interplay between the Rashba and Zeeman effects on the dispersions; the differential conductance results are presented and their features are discussed in Chapter 4 followed by a summary and conclusion of the study in Chapter 5.