Electronic and Photonic Quantum Devices

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Abstract

In this thesis various subjects at the crossroads of quantum mechanics and device physics are treated, spanning from a fundamental study on quantum measurements to fabrication techniques of controlling gates for nanoelectronic components.

Electron waveguide components, i.e. electronic components with a size such that the wave nature of the electron dominates the device characteristics, are treated both experimentally and theoretically. On the experimental side, evidence of partial ballistic transport at room-temperature has been found and devices controlled by in-plane Pt/GaAs gates have been fabricated exhibiting an order of magnitude improved gate-efficiency as compared to an earlier gate-technology. On the theoretical side, a novel numerical method for self-consistent simulations of electron waveguide devices has been developed. The method is unique as it incorporates an energy resolved charge density calculation allowing for e.g. calculations of electron waveguide devices to which a finite bias is applied. The method has then been used in discussions on the influence of space-charge on gate-control of electron waveguide Y-branch switches.

Electron waveguides were also used in a proposal for a novel scheme of carrier-injection in low-dimensional semiconductor lasers, a scheme which altogether bypasses the problem of slow carrier relaxation in such structures.

By studying a quantum mechanical two-level system serving as a model for electroabsorption modulators, the ultimate limits of possible modulation rates of such modulators have been assessed and found to largely be determined by the adiabatic response of the system. The possibility of using a microwave field to control Rabi oscillations in two-level systems such that a large number of states can be engineered has also been explored.

A more fundamental study on quantum mechanical measurements has been done, in which the transition from a classical to a quantum “interaction free” measurement was studied, making a connection with quantum non-demolition measurements.

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List of papers

The thesis is based on the following papers, which will be referred to by their letters:

A A. Karlsson, G. Björk, and E. Forsberg:
"Interaction" (Energy Exchange) Free and Quantum Nondemolition Measurements

B E. Forsberg, J.-O.J. Wesström, L. Thylén, and T. Palm:
Electron waveguide pumped quantum wire far IR laser

C K. Hieke, J.-O.J. Wesström, E. Forsberg, and C.-F Carlström:
Ballistic transport at room temperature in deeply etched cross-junctions

D E. Forsberg and K. Hieke:
Electron waveguide Y-branch switches controlled by Pt/GaAs Schottky gates

E E. Forsberg and J.-O.J. Wesström:
Self consistent simulations of mesoscopic devices operating under a finite bias
(submitted for publication).

F E. Forsberg:
Influence of space-charge on gate-control of electron waveguide Y-branch switches in the coherent regime
J. Appl. Phys. (to be published).

G E. Forsberg, L. Thylén, and B. Hessmo:
Limits to Modulation Rates of Electroabsorption Modulators
(to be submitted).

H E. Forsberg and L. Thylén, Microwave-controlled Rabi-oscillations in two-level systems
(submitted for publication).
Related conference contributions not included in the thesis


List of acronyms

2DEG Two-Dimensional Electron Gas
BDD Binary Decision Diagram
DFB Distributed Feedback Laser
BPM Beam Propagation Method
CCN Controlled Controlled Not
CMOS Complementary Metal Oxide Semiconductor
DOS Density Of States
FET Field Effect Transistor
HEMT High Electron Mobility Transistor
MOSFET Metal Oxide Semiconductor Field Effect Transistor
MOVPE Metal-Organic Vapor Phase Epitaxy
RIE Reactive Ion Etching
QND Quantum Non-Demolition
QPC Quantum Point Contact
QW Quantum Well
VCSEL Vertical Cavity Surface Emitting Laser
YBS Y-Branch Switch
In memory of Lars Henry Forsberg, *16.10.1942 – †27.2.1979
Chapter 1

Setting the scene

Rolf Landauer used to argue that information is a physical and not an abstract entity, referring to the fact that information is invariably tied to the degrees of freedom of whatever physical system you choose to represent the information [1] with. This neatly connects the world of computation and communication with the world of physics, a crossroads of a sorts in which this thesis stands. The binding theme of the subjects treated in this thesis, which in a sense cover a wide range, is the physics of information. Some subjects treat the amount of information which can be transmitted by means of light, others discuss different aspects of how to achieve high-speed computation, while one dwells deep into the obtaining of information, i.e. the physics of a measurement.

In 1965 Gordon Moore predicted that the number of components on a silicon chip would double every year [2]. This he later revised to a doubling every 18 months [3], which is a rate that still holds true even today. This prediction, usually termed ‘Moore’s law’ is in parts self-fulfilling as scientist and engineers in the field deliberately work towards its fulfillment. This is maybe most obviously manifested in the International Roadmap for Semiconductors [4], which is basically a research plan for the semiconductor community. So far, the key to the success of this scaling is the ability to shrink the size of existing devices, i.e. the basic operating principles of the devices remain the same, only the size changes. At present MOSFETs (Metal Oxide Semiconductor Field Effect Transistors) are expected to be extended beyond the 22 nm-node, implying physical gate-lengths of 9 nm, somewhere between the 2010 and 2016 and it is believed that further miniaturization will not be possible to continue somewhere beyond that limit [5]. The reason for this is that although devices have been tiny to the human eye for a long time, it is not until sometime now that electronic devices will start to feel small even for the electrons, with the implication that the quantum nature of the electrons will dominate the device characteristics. This has of course profound effects on the design principles for future electronics devices.
This is then the area where quantum physics meets device design and the driving forces pushing the field forward is both new and interesting fundamental physics as well as practical applications, thus a exciting field. Extensive research is being made in this field and device ideas are abundant, a good review of which can be found in [6]. This thesis partly discusses fabrication and numerical analysis of electron waveguide devices which operate in this interesting regime. The focus of the work has been to go beyond proof-of-concept devices and try to adress issues which will be of importance when such devices are to be implemented in a more realistic setting.

Small size is however not the whole story as every operating device generates heat, thus when packing more and more devices together the issue of power dissiaption becomes very important and potentially limiting. That is, even if you posses the technique to pack a certain amount of devices onto a small area you may be prevented to do so due to the total heat generated. To this end, the electron waveguide device aimed at in some of the papers of this thesis is one which promises extreme low power consumption.

In parallel with the evolution of electronics and computing power we have seen an equally impressive development of the field of optical communications, going through an exponential increase in bit-rate distance product over the years. The approximate starting point can be set to 1970 when loss in optical fibers could be reduced to about 20 dB/km for wavelengths around 1 \(\mu\text{m}\) [7] at the same times as a GaAs-laser lasing continuously at room-temperature was demonstrated [8]. To this field the thesis contributes discussions of a more principal nature concerning speed-limitations in optical communications, focusing on what would be possible within the bounds of physics while deliberately neglecting more practical details of engineering.

In the following chapters the work done in the papers on which this thesis is based are presented and set into perspective by discussing the underlying physics and relating to work done by others in the respective fields. Chapter 2 briefly introduces quantum mechanics and low-dimensional systems. Chapter 3 is concerned with electron transport in electron waveguides as well as devices and logic based on such waveguides. Chapter 4 discusses optical quantum devices with the focus on the speed of lasers and modulators. A lot of the work in the papers is based on computer simulations, and to that end chapter 5 describes the computational methods used. Most of the papers are theoretical in nature, however electron waveguide devices have also been fabricated, and fabrication techniques for such devices are discussed in chapter 6. The thesis ends with the a summary of the original papers and conclusions in chapter 7. All the scientific news of the thesis are found in the original papers with the exception of a device proposal in chapter 3.2.2.

When writing this thesis, my aim has been to make it understandable for an audience wider than those scientists active in the field, as well as keep the tone slightly above the somewhat dry and technical one that usually characterizes scientific papers. That said it is of course unavoidable that some parts will end up somewhat complex.
Chapter 2
Physics for a small world

The size of the various kinds of devices treated in this thesis is such that they are often referred to as *mesoscopic*, implying that they belong to a realm in between the macroscopic world in which we ourselves live and the microscopic world of atoms and elementary particles. Mesoscopic derives from the Greek word *mesos* meaning ‘in the middle’. Being in the middle can always have its problems, and the same apply to the world of mesoscopic physics. The systems considered are generally too large to make a full quantum treatment possible, and yet too small to be a fully classical system. The term *semi-classical* is often used, implying that the description includes a little bit of both quantum and classical physics. In this chapter I will briefly introduce some of the physics that are discussed later on in this thesis.

2.1 Quantum Mechanics Primer

Although the descriptions of mesoscopic systems borrow concepts from both the classical and the quantum world it should be emphasized that the main physical toolbox used is quantum mechanics. Hence an understanding of quantum mechanics is a prerequisite in dealing with mesoscopic systems. The title of this section is of course slightly too ambitious as it would be futile try to give a full description of quantum mechanics in a few short paragraphs. To that end there a vast amount of literature available, e.g. [9], which is a good introductory text or [10], a very good more advanced text. Below I will just state some of the basics of quantum mechanics that will appear later in this thesis, as well as discuss quantum measurements.
2.1.1 Basics

We describe a physical system by a state-vector, which in the Dirac-notation is denoted $|\alpha\rangle$. The observables of the system, i.e. what we can actually measure such as for instance the momentum of an electron, are represented by a hermitian operator, e.g. $\hat{X}$. If we let any operator act on the state-vector, we will achieve information about the state-vector corresponding to the operator and possibly change that state as well. For an operator $\hat{X}$ there exists a special and important class of states, the eigenstates. Letting the operator act on an eigenstate will produce just a number, the eigenvalue (which is real if the operator is hermitian) and leaves it unchanged. Normalized eigenstates form a complete and orthonormal set so we can expand a general state-vector in terms of the eigenstates

$$|\alpha\rangle = \sum_n c_n |n\rangle \quad (2.1)$$

where the expansion coefficient $c_n$ in general is a complex number. This is analogous to the description of the position in Euclidian space, $\vec{r} = x \cdot \vec{e}_x + y \cdot \vec{e}_y + z \cdot \vec{e}_z$, where $\vec{e}_i$ are the unit-vectors. The inner product of two states, $\langle \beta | \alpha \rangle$, is by this analogy equivalent to the scalar product, $\vec{r}_i \cdot \vec{r}_j$, of two vectors.

The position eigenstate $|x\rangle$ is the eigenstate of the position operator $\hat{x}$ with an eigenvalue corresponding to position. The inner product of the position eigenstate and a general state-vector is a function of position

$$\langle x | \alpha \rangle = \psi(\bar{x}) \quad (2.2)$$

that is usually called the wavefunction.

One well-used operator is the Hamiltonian, $\hat{H}$, which gives us the energy of the state, i.e. it is the energy-operator

$$\hat{H} |\alpha\rangle = E|\alpha\rangle \quad (2.3)$$

2.1.2 Example - particle in a box

Let us now look at a simple but important example that is found in most basic texts on quantum mechanics, that of the particle in a box. We consider the problem in one dimension as depicted in Fig. 2.1, the particle can be an electron (which is most relevant for this thesis) and the box we take to be an infinite potential well. The Hamiltonian can then be written as

$$\hat{H} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \quad (2.4)$$

where $\hbar$ is Planck’s constant, $\hbar = 6.63 \cdot 10^{-34} Js$, divided by $2\pi$ and $m$ is the mass of the particle. The potential $V(x)$ is defined such that

$$V(x) = \begin{cases} 
0 & -a \leq x \leq a \\
\infty & |x| > a 
\end{cases} \quad (2.5)$$
Inserting Eq. (2.4) into (2.3) and multiply from the left with the position eigenstate \( \langle x | \)  
$$
\langle x | - \frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) | \alpha \rangle = \langle x | E | \alpha \rangle 
$$
(2.6)
yields 
$$
- \frac{\hbar^2}{2m} \frac{\partial}{\partial x} \psi(x) + V(x) \psi(x) = E \psi(x) 
$$
(2.7)
where \( \psi(x) \) is as defined by (2.2). Eq. (2.7) is the well-known Shrödinger’s time-independent wave equation in one dimension. Solving Eq. (2.7) using the potential (2.5) and the appropriate boundary conditions (i.e. the wavefunction should be a continuous, single-valued function, the derivative of the wavefunction should also be continuous except where there is an infinite discontinuity) gives us an infinite number of solutions:

$$
\psi_n(x) = \begin{cases} 
\frac{1}{\sqrt{a}} \cos \left( \frac{n \pi x}{2a} \right) & n \text{ odd} \\
\frac{1}{\sqrt{a}} \sin \left( \frac{n \pi x}{2a} \right) & n \text{ even} \\
0 & |x| > a
\end{cases}
$$
(2.8)
where \( n \) is a positive integer. The corresponding energy-eigenvalues being

$$
E_n = \frac{\hbar^2 \pi^2}{8ma^2} n^2. 
$$
(2.9)

From this we learn that energy of the particle trapped in the box is quantized, i.e. there is only a specific set on energy-values that the particle can have, namely those given in (2.9). These corresponds the different eigenstates \(|n\rangle\) discussed above and
are sometimes referred to as modes. The constant \(1/\sqrt{a}\) in Eq. (2.8) is a result of the condition that the wavefunction should have the following property:

\[
\int |\psi(x)|^2 dx = 1 \tag{2.10}
\]

or equivalently

\[
|\langle \alpha | \alpha \rangle|^2 = 1 \tag{2.11}
\]

This condition derives from the fact that the \(|\psi(x)|^2 dx\) represents the probability that our particle can be found in the interval \([x, x + dx]\), and as the particle exists somewhere for sure, summing over the whole space should give us unity probability of finding the particle.

### 2.1.3 Dynamics

There are several ways to describe the dynamics of a quantum mechanical system, i.e. to calculate its time-evolution, however throughout this thesis the time-dependent Schrödinger equation is used. The time-dependent Schrödinger equation is written as

\[
\hat{H} |\alpha \rangle = i \frac{\partial}{\partial t} |\alpha \rangle \tag{2.12}
\]

and the general solution is

\[
|\alpha(t)\rangle = \exp \left[ -\frac{i}{\hbar} \int_{t_0}^{t} dt' \hat{H}(t') \right] |\alpha(t_0)\rangle^1. \tag{2.13}
\]

How to implement Eq. (2.13) in numerical calculations will be discussed in chapter 5.

### 2.1.4 Quantum measurements

An important aspect of quantum mechanics is the concept of a measurement. In the quantum world we have to consider that the measurement-apparatus and the object are intertwined, making the measurement will affect the object. Phrasing this mathematically we say that the measurement represents an operator \(\hat{M}\) that acts on the quantum state \(|\alpha\rangle\), and as we have discussed above, letting an operator act on a quantum state generally does something to that state. Take for instance the case of the particle in a box discussed above, we calculated a set of allowed states, the eigenstates \(|\langle n\rangle\rangle\), each with corresponding energy-eigenvalues \(E_n\). In general the state of the particle need not be that of one of the eigenstates, it can be a superposition of eigenstates as stated in Eq. (2.1). But what of the energy? What would we find if we tried to measure the energy of such a superposition?\footnote{This is true when the Hamiltonian commutes with itself at different times, i.e. \([H(t_1), H(t_2)] = 0\), which is the case in all problems discussed in this thesis.}
2.1. Quantum Mechanics Primer

As the particle can only have an energy corresponding to one of the eigen-energies these are the only values we can measure. The measurement will **collapse** the superposition state into one of the eigenstates,

$$\alpha = \sum c_n |n \rangle_{\text{measurement}} \rightarrow |n \rangle$$

(2.14)

and the energy measured is that of the eigen-state the superposition state collapsed to. The measurement is inherently indeterministic since we have no way of knowing before the measurement to which eigenstate the superposition will collapse. The probability of measuring the energy $E_n$ is found from

$$|\langle n | \alpha \rangle|^2 = |c_n|^2.$$  

(2.15)

If the state on which we wish to make our measurement on is in an eigenstate already before the measurement, the state will not be modified and we call this a quantum non-demolition measurement (QND).

A well-known concept from quantum mechanics is the **particle-wave duality**, a quantum object has both wave- and particle-like properties. It easy to visualize an electron as a particle, but later in this thesis we will see how we can describe the currents in small devices be means of wave-transmission. So it is in a sense not meaningful to discuss wether a quantum object is either a particle or a wave, it is both. However, Niels Bohr’s principle of complementarity does state that it is not possible to observe the particle- and wave-like properties of a quantum object at the same time. If we let a quantum object pass through a double-slit and then hit a detection screen behind the slit we will measure a wave-like interference pattern on the screen, much in the same way as in Young’s double-slit experiment (then again, photons are quantum objects as well so this should be expected). If, however, we do the same thing but also measure which of the two slits the object did pass through, then we will see no interference pattern. The interference pattern is of course a wave-like property whereas a particle has to pass through on of the two slits. So, depending on the measurement-setup the electron will display either its wave-like or particle-like properties, both not both.

Making use of this Elitzur and Vaidman [11] proposed an experiment in which the presence of an absorbing object could be detected without absorbing any photons that they called an interaction free measurement. Consider the interferometer in Fig. 2.2, a photon sent in to this have two paths to choose from, the upper and the lower. If we do not measure which path it takes, the photon will show its wave-like character and we can observe interference due to the two paths available. We can set up the interferometer in such a way that the interference is destructive at the upper detector, and thus we will only measure the photons in the lower detector. If we now insert an object into the upper path, the interference is lost since if we measure a photon in one of the detectors we know that the photon must have taken the lower path. What’s more, as the interference is lost the photon can now be detected by both detectors. So if we detect a photon in the upper detector we have gained information about the presence of the absorbing object without any photons...
Chapter 2. Physics for a small world

Figure 2.2. Setup for interaction free detection of an absorbing object using a photon interferometer.

being absorbed by the object. An analogous setup is that of using a cavity [12], which has the advantage of having higher efficiency in terms of the probability of finding the object without photon absorption. In Paper A, the nature of such interaction free measurements were considered for cases when the absorbing object was not a classical but a quantum object. It should be stressed that the term interaction free can be somewhat misleading, the detected object do interact with the measurement apparatus, the key point is that the object is detected without the photon being absorbed and thus the term energy-exchange-free measurements is more accurate and also often used [13].

2.2 Low-dimensional systems

Normally we perceive to world we live in as a three-dimensional world, as does an electron in a large crystal. However, if you stand in the middle of a field you realize that you are actually confined to two spatial directions, you can only move in the left/right- or forward/backward-directions. Similarly, we can reduce the freedom
2.2. Low-dimensional systems

of movement for an electron in a crystal to two, one or even zero-dimensions. This then is what we mean by a low-dimensional system, it is a physical system in which a particle, be it an electron, hole (the absence of an electron), phonon (a quantized lattice-vibration) or a photon is confined to ‘live’ in a world with fewer dimensions than three. The possibility to confine particles into two-, one- and zero-dimensional system opens up a vast field for constructing novel kinds of devices for electronic, optical and optoelectronic applications. It also creates a very useful toolbox for fundamental study of quantum mechanical phenomena. How to actually create such a confinement for electrons will be discussed in chapter 6.

In the parts of this thesis where such systems are concerned it is those for electrons, so let us discuss some of the properties of such low-dimensional electron systems. Even further, we will mainly be discussing the properties of the electrons in the conduction band. The Hamiltonian for such an electron can be written as

\[ \hat{H}_{\text{eff}} = \frac{1}{2m^*} \left( i \hbar \nabla + eA \right)^2 + U(\vec{r}) + E_c, \]  

where \( A \) the vector potential, \( e \) the electron charge, \( U(\vec{r}) \) is the potential energy due to space-charge etc. and \( E_c \) is the conduction band energy, which in general is spatially dependent. This is referred to as the single-band effective-mass description as the lattice-potential of the crystal is incorporated through the concept of the effective mass, \( m^* \). The wavefunctions corresponding to this Hamiltonian will actually be envelope functions of the ‘true’ wavefunction omitting the rapid oscillations due to the lattice-potential. This is usually an adequate description for electrons in the conduction band at low fields.

Now, consider the particle in a box discussed in 2.1.2, which can represent confinement of the electron in one direction. In such a case, the electron can move freely only in the directions perpendicular to the well, and thus we have a two-dimensional system. In an actual physical system the confining potential would of course not be infinite, and the well will also have some finite width, which in turn means that the wavefunction of the electron has some extension in that direction as well. So strictly speaking this is not a true two-dimensional system but a quasi-two-dimensional system, but the term quasi is usually omitted for brevity. Systems like these are usually called quantum wells.

In a similar fashion we can then further confine the electron in yet another direction and there now only exists one spatial direction in which the electron is free to move in. The wavefunction for such an electron can be written

\[ \psi(\vec{r}) = \frac{1}{\sqrt{L}} \phi_{n,m}(x,y) e^{ik_z z} \]  

where \( L \) is the length of the one-dimensional conductor over which the wavefunction is normalized. \( \phi_{n,m} \) is a two-dimensional wavefunction calculated in the same manner as the particle in a box problem above, representing different modes. Such a system is then of course a quasi-one dimensional system, often referred to as a quantum wire or electron waveguide. The latter term is due to the fact there exists
strong analogies between the transport of electrons in such a system and the transport of electromagnetic waves in waveguides as treated in the field of microwave engineering [14]. If the wire is very short it is usually referred to as a quantum point contact. The transport of electrons in electron waveguides has more similarities to a wave-propagation problem that that of classical electrical currents, as will be seen in chapter 3. Reducing the electrons in the last dimension as well completely traps them spatially in space, and we have a quasi-zero dimensional system, often referred to as a quantum box/dot or artificial atom.

Electrons, being fermions, are not very sociable particles as they obey the Pauli exclusion principle, which states that no two electrons can occupy the same state. This makes it necessary for us to be able to do some bookkeeping of which states the electrons actually occupies. The way we do it is by using a function, $D(E)$, which gives the density of available states per energy. $D(E)$ is usually called just the density of states or DOS for short. The DOS does however only tell us the number of available states, not which ones are actually occupied by an electron.

The way the electrons organize themselves is to fill up the available states with the lowest energy first and then work their way upwards. At zero temperature all states will be filled up to an energy called the electrochemical potential, $\mu$. If the temperature is higher than zero (which it usually is) this is not true, the states are then populated according to the Fermi-Dirac distribution function

$$f_0(E) = \frac{1}{1 + \exp[(E - \mu)/k_B T]}$$  \hspace{1cm} (2.18)

where $k_B = 1.38 \cdot 10^{-23} J/K$ is Boltzmann’s constant, $T$ the temperature and $\mu$ the electrochemical potential. The Fermi-Dirac distribution smears the unpopulated and populated states over an energy-range that is comparable to the thermal energy.
2.2. *Low-dimensional systems*

$k_B T$. The total number of electrons in our system can be found by the integral

\[ n_s = \int D(E) f_0(E) dE. \]  \hspace{1cm} (2.19)

The DOS tells a lot about the properties of our system, thus one of the easiest ways to understand why low-dimensional systems have such special qualities compared to each-other and three-dimensional systems is to compare their DOS as is done in Fig. 2.3.
Chapter 3

Electron waveguide devices

Electron waveguides as discussed in the previous chapter provides a coupling between the worlds of quantum mechanics and engineering. In such devices, the wave nature of the electron dominates and we turn to quantum mechanics to calculate the relationship between currents and potentials. At the same time, continued scaling of logic circuits are shrinking semiconductor components into sizes of the same order of magnitude as the electron waveguide devices thereby making quantum effects an important factor in the engineering of logic circuits.

3.1 Current and conductance

From high-school physics we know that the relation between current and voltage is expressed in the well-known Ohm’s law, \( U = R \cdot I \), where \( U \) is the voltage, \( I \) the current and \( R \) the resistance. The resistance \( R \) depends on the resistor geometry and the conductivity \( \sigma \), which is a macroscopic material property. The voltage amounts to an electric field across a conductor that accelerates the electrons, however, when moving through the conductor the electrons are constantly scattered by impurities and this scattering counters the acceleration. The net effect is that the electrons on the average are moving at a constant speed in a random fashion in the direction of the acceleration. This is called the drift-current, and is what Ohm’s law describes. A difference in concentration of electrons across the sample, a concentration gradient, will also trigger the electrons to move in a similar fashion. This is the diffusion-current and together they constitute (not surprisingly) the drift-diffusion-current.

The drift-diffusion description derives from the semi-classical Boltzmann equation and is adequate to describe currents and electron motion in traditional semiconductor devices and is described in most basic textbooks on semiconductor physics, e.g. [15]. However, if the size of a device is made sufficiently small this description
will not hold. This is due to the fact that some assumptions made when deriving the standard results of conduction from the Boltzmann equation, such that the electron should move as a classical particle between scattering events and that these are independent, are not valid in such small devices. Clearly some new physics is needed to describe the transport properties of electrons in such devices, and the way to do it is to turn to a quantum mechanical description. One very successful and intuitively appealing description is the Landauer-Büttiker formalism [16] in which the transport properties of electrons are described in terms of wave-transmission applied to the wavefunction of the electron. But before we describe that let us first discuss different types of scattering and their influence on the electron transport.

3.1.1 Scattering and length-scales

Scattering of electrons can be either elastic or inelastic, the difference between the two is that the electron loses some of its kinetic energy in the inelastic case which it does not in the elastic. What’s more, inelastic scattering randomizes the phase of the electron wavefunction whereas elastic scattering does not. In short we can say that elastic scattering is due to stationary scatterers such as impurity atoms and inelastic scattering is due to moving scatterers such as other electrons or phonons.

The distinction of the types of scattering connects to two important length-scales, the elastic mean free path (often referred to as just the mean free path) and the length over which the electron loses its phase. The mean free path is simply the average distance an electron travels between two elastic scattering events, while the length over which it loses its phase is not as simply defined. This can be understood if we compare the time it takes for the electron to lose its phase memory, the phase relaxation time $\tau_{\phi}$, and the time between two elastic scattering events, $\tau_e$. If $\tau_{\phi}$ is less or of the same order of $\tau_e$ then the length over which the electron loses its phase is defined as the length between two inelastic scattering events, or

$$l_{in} = v_f \tau_{\phi}$$

where $v_f$ is the Fermi-velocity, the speed at which the most energetic electron travels at. However, if $\tau_{\phi} \gg \tau_e$ then a large number of elastic scattering events occur while the electron keeps its phase memory, the motion of the electron is then diffusive and the length over which the electron loses its phase is

$$l_{\phi} = \sqrt{D \tau_{\phi}}.$$  \hspace{1cm} (3.2)

where $D$ is the diffusion coefficient. The effective phase relaxation length can thus be either the inelastic scattering length, $l_{in}$, or the phase coherence length, $l_{\phi}$ depending on the relation of $\tau_{\phi}$ and $\tau_e$ [17, 18].

Now we can define what is meant by sufficiently small as discussed above. If the dimensions of the conductor are much larger than any of the scattering lengths, then the Boltzmann equation can be used. If on the other hand, the mean free path and inelastic scattering length are larger than the size of the device, then the quantum
3.1. Current and conductance

Figure 3.1. Electron waveguide connecting two reservoirs.

state of the electron extend throughout the conductor and the Boltzmann equation cannot be used. Using the wave-like properties of the electron the conductance of the device can be determined. By the complementary view of electrons as particles we can say that the electron shoots through the device in a ballistic trajectory, hence the term *ballistic transport* is commonly used. This situation can quite easily be achieved at low temperatures in high-mobility semiconductor devices, but transmission characteristics that are partially ballistic have been measured even at room temperature, see e.g. [19] and Paper C of this thesis.

A much different type of transport is that found in the weak localization regime. This can occur in low-mobility semiconductor devices in which the phase coherence length is larger than the sample size which in turn is larger than the mean free path, i.e. $l_{\phi} \gg l \gg l_e$. In this regime quantum corrections to the conductance due to interference between the different scattering events must be taken into account, see e.g. chapter 5 in [17].

3.1.2 Describing conductance as transmission

Consider an electron waveguide connected between two reservoirs as schematically shown in Fig. 3.1 and assume that the size of the waveguide is such that we are in the ballistic transport regime. We can then expect an electron to travel uninterrupted through the waveguide and might ask ourselves what the conductance would be. How about an infinite conductance? Given the fact that the resistance of a conductor stems from the elastic and inelastic scattering of which there are none, it might seem reasonable to guess that the resistance would be zero (and thus the conductance infinite). This is however not true, and we shall see below why it is so.

Recall from 2.2 that an electron waveguide is in essence a one-dimensional system and that the wavefunction of the electron is quantized in the directions perpendicular to the length of the waveguide. We know that $n$ electrons per unit length moving with velocity $v$ carry a current equal to $env$ where $e$ is the electron charge. The electrons in mode $m$ moving from left to right in the electron waveguide have
Chapter 3. Electron waveguide devices

a group-velocity
\[ v_g = \frac{1}{\hbar} \frac{\partial E}{\partial k_m} \] (3.3)

and a density of states
\[ D_m = \frac{1}{2\pi} \frac{\partial k_m}{\partial E}. \] (3.4)

We generalize a little bit and allow for elastic scattering and assume that the probability for electrons injected into mode \( m \) from the left reservoir to traverse to the right reservoir is \( T_m \). The contribution from these electrons to the current is then (including spin-degeneracy)
\[ I_m^+ = 2 \times \int v_g D_m T_m f^+(E) dE = \frac{2e}{\hbar} T_m \int_{\varepsilon_m}^{\infty} f^+(E) dE \] (3.5)

where \( f^+(E) \) is the Fermi-Dirac function and \( \varepsilon_m \) is the bound energy-eigenvalue of mode \( m \). We can calculate a equivalent expression for the electrons moving from right to left, \( I_m^- \) and then find the net-current in mode \( m \) to be
\[ I_m = I_m^+ - I_m^- = \frac{2e}{\hbar} T_m \int_{\varepsilon_m}^{\infty} \left[ f^+(E) - f^-(E) \right] dE. \] (3.6)

In the zero-temperature limit the integral of the Fermi-Dirac function is just a step-function so it is easy to see that the integration in (3.6) is just \( \mu^+ - \mu^- \). This is also true at finite temperatures, and thus we can write the current as
\[ I_m = \frac{2e^2}{\hbar} T_m U \] (3.7)

where \( U = (\mu^+ - \mu^-)/e \) is the applied voltage between the two reservoirs. The total current is just the sum of the currents in the populated transverse modes, and so total conductance of the waveguide is
\[ G = \frac{2e^2}{\hbar} \sum_m T_m. \] (3.8)

Thus even for a waveguide in which the transmission probabilities are unity (i.e. no scattering at all) the conductance of the device is finite, it is a constant, the fundamental unit of conductance, \( G_0 = 2e^2 / \hbar \simeq 77 \mu S \), times the number of occupied modes. This was a fairly disputed point (see [20] and references within) before it was experimentally verified in 1988 in two independent set of experiments [21, 22]. It is interesting to note that Landauer as early as 1957 published a paper in which he discussed the resistance in terms of reflection probabilities [23], the crucial point being that in the absence of inelastic scattering it must be possible to express the global conductances of a device in terms of a scattering matrix. Later Büttiker used simple counting arguments as above to formulate a description of
3.1. Current and conductance

the conductance of a general multi-port device [16] and in [24] it was shown that those results follow from microscopic theory using a rigorous derivation based on the Kubo-formula.

But why is the conductance finite? It is important to note the we are discussing the global conductance which connects the currents through the device with the potential differences in the reservoirs. The reservoir has in a sense an infinite number transverse modes whereas the the waveguide has but a few. Consequently most electrons impinging on the waveguide from the reservoir are reflected, simply stated, by the mere fact that there is not room enough for all of them in the waveguide. Thus there is a resistance that stems from the interfaces of the reservoirs and the device, and thus the conductance is finite.

Eq. (3.8) is actually only valid in what is called the linear-response regime, in which the transmission probabilities $T_m$ are independent of energy and unaffected by the applied bias. However, in general, this is not true, i.e. $T_m = T_m(E)$. At zero temperature the variation stems from the geometry of the device as well as impurities etc. and the transmission probabilities change rapidly with energy. The correlation energy $\varepsilon_c$ is a measure of how rapidly $T_m(E)$ varies with energy, i.e. large correlation energy means slow variation in energy. A temperature above zero will smear the transmission probabilities’ energy-dependence and thus increase the energy-interval in which the response can be said to be linear. The general criterion for the response to be linear is then [17]

$$\Delta \mu + k_B T \ll \varepsilon_c$$

(3.9)

where $\Delta \mu$ is the difference between the electrochemical potentials in the reservoirs.

For a general multi-port device such as in Fig. 3.2 which is connected to $N$ reservoirs the relation between the currents and electrochemical potentials can be

Figure 3.2. General multi-port device connected to $N$ number of reservoirs.
Figure 3.3. Electron waveguide Y-branch switch; electrons injected into the stem are deflected into either of the two branches by means of the side-gates.

Expressed as

\[
\begin{pmatrix}
I_1 \\
I_2 \\
\vdots \\
I_N
\end{pmatrix} = \frac{2e}{h} \int (E - T) \cdot \begin{pmatrix}
f_1(E) \\
f_2(E) \\
\vdots \\
f_N(E)
\end{pmatrix} dE.
\]  

(E is the identity matrix and T is the transmission probability matrix. The elements of T, \( T_{ij} \) are given by \( T_{ij} = \sum_{mn} |s_{ij,mn}|^2 \), where \( |s_{ij,mn}|^2 \) relates the complex amplitude of an outgoing electron wave \( \beta^-_{i,m} \) in mode \( m \) in waveguide \( i \) to that of the incoming electron wave, \( \beta^+_{j,n} \) in mode \( n \) in waveguide \( j \).

\[
\beta^-_{i,m} = \sum_{jn} s_{ij,mn} \beta^+_{j,n}
\]

Thus we see that within the Landauer-Büttiker formalism, transport calculations in electron waveguide devices is in the end a matter of calculating the s-parameters of the structure. This is however not a trivial problem and there are a number of methods to do this, one which is proposed in Paper F, which will be discussed in some further detail in chapter 5.2.

3.2 Electron waveguide Y-branch switch (YBS)

Utilization of the wave-like properties of the electron as a basis for functional devices to be used in logical circuitry has been discussed ever since the first demonstrations of quantized conductance in quantum point contacts (QPCs) [21, 22]. Electron waveguide devices have generally been accepted as a candidate class of devices for
ensuring continuation of Moore’s law beyond the scaling of present day CMOS-technology [6]. The QPC can in itself act as a field-effect transistor (FET), there is actually no difference in principle between the two, it is basically a question of size. The possible additional functionality of a QPC lies in the transverse modes, which could serve as a basis for multi-valued logic, i.e. logic based on more states than two as in conventional binary logic.

Several devices have been proposed, such as an electron waveguide directional coupler [25, 26] and the quantum stub-transistor [27]. Related is also the use of an Aharonov-Bohm interferometer for the same purpose [28]. However, while elegant demonstrations of the wave-like properties of the electron these devices all share the shortcoming of having a sinusoidal response to an applied gate-voltage. This makes it very dubious if they could ever be used as building blocks for future logic as they are extremely sensitive to defect-tolerances in large-scale integration.

The Y-branch switch (YBS) [29] is an electron waveguide device as well, but with the advantage that the response is monotonous. The YBS is formed by connecting three electron waveguides in the shape of a Y as shown in Fig. 3.3. Electrons entering the stem of the device are deflected to either of the two stems by applying a gate-bias across the device. This characteristic is of course not dependent on the wave nature of the electron, the response would be similar for a ‘classical’ YBS, however it can be shown that if the the YBS operates in the single-mode coherent regime the theoretical limit to the required voltage necessary to achieve switching is limited by [30]

$$\Delta V_S \geq \frac{\hbar}{e\tau_{tr}},$$

(3.12)

where $\tau_{tr}$ is the transit-time of the electron through the switching region of the YBS. This means that there is no thermal limit for switching as there is for an FET. Intuitively this can be explained by the fact that electrons entering the YBS need not be stopped as they do in an FET, they need merely be deflected. This is a strong argument for the YBS when it comes to large-scale integration as heat generation of the devices is one the key issues, the less heat the devices generate, the more densely they can be packed.

Ballistic switching is an altogether different mode of operation of the YBS [31, 32, 33]. By leaving the stem floating and changing the voltage of the two stems it turns out that stem-voltage will always follow the more negative of the two voltages making it effectively a rectifying device. This is a multi-mode ballistic effect that is still observable at room temperature. Interestingly enough, such effects have also been seen in carbon-nanotube Y-junctions [34].

### 3.2.1 Space-charge effects in the YBS

Early simulations of the characteristics of the YBS showed that if designed properly the reflection of electrons injected into the stem was negligible [35], which meant
that in the absence of a magnetic field the transmission matrix of the YBS was
dependent of only one single parameter, $\gamma$:

$$T_Y = \begin{pmatrix}
0 & \frac{1+\gamma}{2} & \frac{1-\gamma}{2} \\
\frac{1+\gamma}{2} & \frac{(1-\gamma)^2}{4} & \frac{1-\gamma^2}{4} \\
\frac{1-\gamma}{2} & \frac{1-\gamma^2}{4} & \frac{(1+\gamma)^2}{4}
\end{pmatrix}. \quad (3.13)$$

The same simulations as well as experimental results [36] suggested that the switching-
parameter $\gamma$ could be approximated as

$$\gamma = \tanh \left( \eta_g \frac{\Delta V_g}{\Delta V_S} \right). \quad (3.14)$$

$\eta_g$ is a measure on how well the potential difference inside the YBS at the junction
follows the voltage difference of the gates, $\Delta V_g$. The switching-voltage $\Delta V_S$ is a
measure of the response of $\gamma$. In [37] the effects of space-charge in the YBS were
first considered and the point made was that, when switching electrons from the
stem to e.g. the left branch one creates a pileup of charge in the left branch which
in turn creates an internal field between the the branches. This field is directed such
that it will oppose the intended switching. One should then modify the switching-
parameter in order to take this into account

$$\gamma = \tanh \left( \eta_g \frac{\Delta V_g}{\Delta V_S} + \eta_{sg} \frac{\Delta \mu_{23}/(-e)}{\Delta V_S} \right). \quad (3.15)$$

As Eq. (3.15) predicts that switching can be achieved even in the absence of an
applied gate-bias, $\Delta V_g = 0$, this was termed self-gating. $\eta_g$, the self-gating ef-
fi ciency is, in the same manner as $\eta_g$ a measure how well $\gamma$ follows the difference in
electrochemical potential in the two branches $\Delta \mu_{23}$. A crucial point is the relative
magnitudes of $\eta_g$ and $\eta_{sg}$ and in [37] it was argued that the self-gating would be the
dominant switching mechanism. It may be possible to ‘wash out’ the self-gating
mechanism by using a sufficiently large gate-bias, however that would defeat one of
the main arguments for the YBS, which is low-power switching and cascadeability.

Paper F discusses the effects of space-charge further, where it is argued that
the influence of space-charge on the switching of an YBS cannot be modelled
using a single-parameter description as done in [37]. The reason being that a single-
parameter description rests on a transmission probability matrix independent of en-
ergy, however the charge distribution depends on all electrons in the device meaning
that one needs to consider an energy-dependent transmission probability matrix.
Self-consistent simulations also showed a switching behavior more complex than
can be described by a single-parameter description. This could help explain as to
why self-gating has not been observed experimentally despite repeated efforts [38].
The attempts to verify it did however curiously enough lead to the discovery of the
ballistic switching effect.
3.2. Electron waveguide Y-branch switch (YBS)

3.2.2 Logic using the YBS

One of the first questions concerning any device is ‘Can we design a logic circuit based on this device?’ Concerning the YBS the first answer came in [39] where an inverter, NAND- and NOR-gates based on the YBS were proposed. These gates mimics the functionality of equivalent gates in CMOS-logic, however offer the advantage of compact design as well as reduced power dissipation since they are based on YBSs. Fig. 3.4 shows the design of one of the proposed inverters as well as the same gate fabricated in an AlGaAs/GaAs heterostructure. In a recent paper the ballistic switching effect in the YBS have been utilized to construct a NAND-gate [41].

As one of the two main arguments for the logic gates proposed in [39] is the low energy-dissipation we should consider the implications of the self-gating effect on these gates. This was done in [42] and the conclusion was that if the self-gating efficiency $\eta_{sg}$ is of the same magnitude or larger than the gate-efficiency $\eta_g$ as was argued in [37], then the gates will not function as proposed. The simulations of Paper F do, however, show that for low electrochemical potentials in the reservoirs, i.e. low electron concentrations in the YBS, it can still function as originally proposed in [29] and thus also save the functionality of the logic gates of [39]. The prize one has to pay is reduced speed since low currents take longer to charge capacitive couplings. This should not be very surprising as there is in general a trade-off between speed and power.

Logic circuitry based on MOSFETs is however very competitive and it seems very doubtful if convectional logic based on devices such as the YBS will offer such a significant advantage to motivate the costs of transferring to a whole new technology. It has even been suggested that as long as we are considering computation in...
In view of this let us discuss some possibilities beyond conventional logic that exists for the YBS. One very interesting idea as how to construct logic is the binary-decision diagram (BDD). The use of BDDs is actually an analytical tool for circuit designers, but as was proposed in [44] one can also use the diagrams as a layout for physical devices. By use of such devices an alternative kind of logic can be constructed and they also have an advantage in that they are not dependent on fan-out in the same way as conventional logic. The YBS is a very suitable device for the realization of BDDs, and impressive work has been done in the group of Hasegawa at Hokkaido University to construct such BDDs using a honeycomb-structure incorporating YBS-like switching devices, see e.g. [45].

One could also conceive using YBSs to design a controlled controlled not-gate (CCN) as proposed in Fig. 3.5, which in the same manner as a NAND-gate can be used as the single building block from which all types of logic can be constructed. The CCN-gate is however a reversible gate meaning that one can always reconstruct the input from the output. If you can construct a reversible computer you have constructed a computer that can operate with zero energy-loss. The drawback is of course that such a computer would have to operate infinitesimally slowly which may be slightly impractical, however the point is that you have constructed a computer which can have an arbitrarily small energy-loss [46].

![Figure 3.5. Proposal of a CCN-gate based on three YBSs.](image-url)
Chapter 4

On the speed of lasers and modulators

The physics and technology of lasers is a highly interesting discipline of applied physics in its own right, a thorough discussion on the subject can be found in [47]. There exists a wide variety of lasers systems, e.g. solid-state lasers, gas-lasers, organic-dye lasers and semiconductor lasers, but the basic working principle is the same for all of them. Consider a system with two distinct energy levels, electrons making a transition from the upper to the lower level can emit its excess energy in form of a photon. The transition will occur either spontaneously or it may be stimulated by a passing photon that has an energy matching the energy difference between the two levels. The photon emitted by stimulated emission differs from the spontaneously emitted photon in that it is basically a copy the photon that stimulated the emission. It has not only the same energy but the same phase and propagation direction. If we then place this system in an optical resonator whose resonance frequency matches the frequency of the photons, and let a small portion of the photons escape one of the mirrors. Out will come a beam of phase-coherent monochromatic light, i.e. laser-light.

A large and commercially important class of lasers is semiconductor lasers of which there exists a large variety. These are used in a wide area of applications, e.g. as key-components in fiber-optical communication systems. Confinement of electrons into low-dimensional systems by means of semiconductor heterostructures (see chapter 6) and additional fabrication techniques allows for the fabrication of laser structures such as e.g. the quantum well (QW) laser [48], distributed feedback (DFB) laser [49, 50], vertical cavity surface emitting laser (VCSEL) [51] and the quantum cascade laser [52].

Intimately connected to the generation of laser-light are techniques for modulation, i.e. the ability to change some characteristic of the laser-light as a function of time in a controlled manner. By use of modulation we can encode information
Chapter 4. On the speed of lasers and modulators

onto our beam of laser-light so that we can use it in communication systems, e.g. for digital communication we can represent the 0's and 1's by turning the light off and on.

4.1 Carrier injection

In order to get stimulated emission, we need electrons in the upper level. This may seem like a trivial point, but a photon that can stimulate a transition might as well be absorbed, i.e. an electron makes the transition from the lower to the upper level, and the probability for absorption to occur is equal to that of a stimulated emission. In a steady state the absorption and stimulated emission rates are proportional to that probability times the number of electrons in the respective level. Consequently, if we want lasing to occur we need more photons emitted than absorbed, i.e. we want \( N_2 > N_1 \), where \( N_2 \) and \( N_1 \) are the number of electrons in the upper and lower level respectively. This state of affairs, called population inversion, does not occur naturally, i.e. we have to somehow artificially create the situation. In semiconductor lasers this can be done be means of an electrical current. Without considering the details of the design, consider the simple model of a quantum well inter-band laser as depicted in Fig. 4.1. By applying an electric field across the well the conduction band is tilted and electrons will move downhill in the slope creating a current. Coming to the well, they may fall into the well and we can create a population inversion. If we now want to modulate the laser we can do this by simply turning the current on and off. With the current on, we are supplying the upper level in the well with electrons and lasing can occur. Turning the current off cuts of the supply of electrons and the lasing ceases.

Generally, the electrons are injected into a level far above the upper of our two levels concerned with the stimulated emission process, and thus the electrons need first of all to relax down to that level. In any transition, energy and momentum have to be conserved as well as transition rules be obeyed. Due to the low number of phonons and orthogonality of carrier states in low-dimensional lasers it was predicted that the energy relaxation would be inefficient [53, 54], making such lasers less promising in terms of speed and luminescence than was originally expected. This was dubbed ‘the phonon bottleneck problem’ and has been debated up to date (for recent discussions on the subject see e.g. [55, 56]). The debate has partly concerned mechanisms that seem to limit the effect of this ‘phonon bottleneck’, such as multi-phonon processes [57], Auger-like mechanisms [58], defect-state related relaxation [59].

In response to this, and the fact that the maximum bandwidth is also expected to be limited by slow carrier capture [60], i.e. difficulties to actually get the electrons to fall into the well, Paper B proposed a novel way to inject electrons into low-dimensional lasers. Here the time-consuming relaxation process was circumvented in maybe the most obvious way, the electrons are directly injected into the
specifically desired state. This can be done by coupling an electron waveguide to a quantum wire/dot in a clever way.

4.2 Modulation

Modulation achieved by turning the driving current of a semiconductor laser as discussed above is in general referred to as direct modulation. As with laser-types, modulation techniques come in many flavors, other modulation-schemes besides direct modulation are internal modulation and external modulation, referring to modulators operating inside and outside the resonant laser cavity. Modulation can be achieved by changing the amplitude, phase, polarization, direction or frequency of the light. The realization of any these types of modulation can again be done in a number of ways, amplitude modulation can e.g. be achieved by controlling the absorption coefficient in the modulator. By control of the refractive index we can achieve phase, directional, polarization and frequency modulation [61].

Modulation speeds continuously increase, see e.g. [62], partially as a response to the ever increasing demand for communication bandwidth due to data transmission on the internet and increased wireless communications. Due to this it would be interesting to attempt a discussion on what can be conceived as the ultimate limits of modulation speed. An intuitive, although maybe not fundamental, upper limit for modulation would be that of the optical frequency in itself, as it would be ambiguous to discuss modulation at speeds higher than this. But are there any other limits? In Paper G such a discussion is attempted by discussing a quantum mechanical system that models many modulator types, as opposed to more ‘engineering’-type considerations such as RC time-constants and walk-off [63]. The basic assumption made is that the upper limit of modulation is defined by the requirement that the response of the electron wavefunction to the modulation has to be clearly defined. I.e. the response should be adiabatic. A slit-operator method (as discussed in chapter 5) is used to study this wavefunction-response numerically and it is found that the modulation rate is limited by the validity of the adiabatic approximation.

![Figure 4.1. Quantum well laser without(left) and with (right) an applied electric field.](image-url)
An interesting spin-off to the simulations of the wavefunction response was found. It was discovered that in an asymmetric quantum well it is possible to control the Rabi-oscillations by use of a microwave field thus making it possible to engineer a large number of different states. This is discussed in further detail in Paper H.
Chapter 5

Computer simulations

The use of computer simulations is a powerful tool to understand and visualize a physical problem (and many other problems as well). Computational techniques exist in abundance, and all of them have their own special set of pros and cons. In the work on which this thesis is based, two different techniques are used, split operator methods and a self-consistent Schrödinger-potential simulation. Here these two methods are described in a general fashion, omitting details such as discretization and most questions regarding the actual implementation of the methods in the form a computer program. First we discuss how to calculate the time-evolution of a quantum system by use of split-operator methods, and then a self-consistent method to calculate the potential and charge density distribution of mesoscopic devices is described. Self-consistent simulation methods for quantum systems are common, however this method, which is described in detail in Paper F, takes into account the possibility to apply a finite bias to the device by using an energy-resolved charge density distribution calculation, which to my knowledge is unique.

5.1 Split-operator methods

Frequently we are interested to know how a quantum system evolves in time, that is, we wish to calculate the time-evolution of the system. As was stated in chapter 2.1, the time-evolution of a quantum system is in general described as

\[ |\alpha(\vec{r}, t)\rangle = \exp\left[ -\frac{i}{\hbar} \int_{t_0}^{t} dt' \hat{H}(x, t') \right] |\alpha(\vec{r}, t_0)\rangle \]

(5.1)

where \( \hat{H}(x, t) \) is the Hamiltonian. For most systems it is either difficult or impossible to calculate an algebraic solution to Eq. (5.1), and thus we turn to numerics.
For a Hamiltonian of the form

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(\vec{r}, t)$$  \hspace{1cm} (5.2)

where $\hat{p}$ is the momentum operator and $\hat{V}$ is the total potential, we can then write Eq. (5.1) for a small time-step $\Delta t$ as

$$|\alpha(\vec{r}, t + \Delta t)\rangle = \exp \left[ -i \frac{\Delta t}{\hbar} \frac{\hat{p}^2}{2m} - i \frac{\Delta t}{\hbar} \hat{V}(\vec{r}, t + \frac{\Delta t}{2}) \right] |\alpha(\vec{r}, t)\rangle = e^{\hat{P}} e^{\hat{Q}} |\alpha(\vec{r}, t)\rangle.$$  \hspace{1cm} (5.3)

Where define the kinetic and potential exponentials are defined as

$$\hat{P} = -i \frac{\Delta t}{\hbar} \frac{\hat{p}^2}{2m}, \quad \hat{Q} = -i \frac{\Delta t}{\hbar} \hat{V}(\vec{r}, t + \frac{\Delta t}{2}).$$  \hspace{1cm} (5.4)

In order to be able to calculate this numerically we need to fractally decompose (or split, hence the term split-operator) the exponential. This however, poses a problem as, in general, for two operators $\hat{A}$ and $\hat{B}$,

$$e^{\hat{A} + \hat{B}} \neq e^{\hat{A}} e^{\hat{B}},$$  \hspace{1cm} (5.5)

if $\hat{A}$ and $\hat{B}$ do not commute. So in general we will get an error in our calculation, a problem of course, but one we can work our way around. We need to know how large the error is and how to minimize it. If we were to decompose Eq. (5.3) as in Eq. (5.5) the error would be of second order in $\Delta t$, i.e. $O(\Delta t^2)$. By doing the decomposition a little more clever we can reduce the error. If we were to do the decomposition as follows

$$e^{\hat{P} + \hat{Q}} \approx e^{\hat{Q}} e^{\hat{P}} e^{\hat{Q}}$$  \hspace{1cm} (5.6)

or

$$e^{\hat{P} + \hat{Q}} \approx e^{\hat{P}} e^{\hat{Q}} e^{\hat{P}}$$  \hspace{1cm} (5.7)

then the error will instead be $O(\Delta t^3)$, a significant improvement. Whether we choose to decompose as in Eq. (5.6) or Eq. (5.7) depends on the problem at hand and how we choose to implement it (a comparative study of these two decompositions as well as other methods of computing the time-evolution was done in [64]). By choosing even more intricate decompositions the error can be made arbitrary small, and a general method of how do calculate these decompositions is outlined in [65]. Normally however, the decompositions (5.6)-(5.7) will suffice for most problems.

Inserting on of the two decompositions (5.6) or (5.7) in Eq. (5.3) it is now possible to numerically calculate the time-evolution by successive application of these compound operators on the initial state of our system, $|\alpha(\vec{r}, t_0)\rangle$:

$$|\alpha(\vec{r}, t)\rangle = e^{\frac{\Delta t}{2}} e^{\hat{P}} e^{\frac{\Delta t}{2}} e^{\hat{Q}} e^{\frac{\Delta t}{2}} e^{\hat{P}} e^{\frac{\Delta t}{2}} e^{\hat{Q}} e^{\frac{\Delta t}{2}} |\alpha(\vec{r}, t_0)\rangle = e^{\frac{\Delta t}{2}} e^{\hat{P}} e^{\hat{Q}} e^{\hat{P}} e^{\hat{Q}} e^{\hat{P}} e^{\hat{Q}} e^{\hat{P}} |\psi(\vec{r}, t_0)\rangle.$$  \hspace{1cm} (5.8)

Notice how we can lump two $e^{\frac{\Delta t}{2}}$ exponentials together and thus reduce the number of computational operations considerably (from $3N$ operations to $2N + 2$ for $N$ time-steps).
Now, the actual implementation of Eq. (5.8) takes some further consideration which we will discuss very briefly. Applying the potential exponential onto the state is basically a complex multiplication, and is thus simply done. The kinetic exponential on the other hand involves a differentiation. One way to handle this is to use the Fourier-transform since in the Fourier-plane a differentiation corresponds to a multiplication of the wave-vector. This approach has been widely used for optical problems, and as such been named the beam-propagation method. In [66] it was applied to the Schrödinger equation and has since been used extensively for quantum dynamical problems. The beam-propagating method (BPM) applied to electron waveguide devices was developed by Palm [29, 67] and this was used in the simulations done in Paper B and Paper C.

The use of the Fourier-transform does however have its drawbacks; mainly that it does not handle abrupt potentials very well. Thus if the problem at hand does include abrupt potential-profiles we should consider some other approach for kinetic exponential, allowing us to stay in real space. We can do this by using a fractional approximation of the exponential known as Cayley’s form

\[ e^Q = e^{-i \frac{\hbar}{2m} \hat{p}^2} = e^{i \Delta t \frac{\hbar}{2m} \nabla^2} \approx 1 + i \Delta t \frac{\hbar}{2m} \nabla^2 / 4m. \]

Using this approximation we can construct an efficient method to calculate Eq. (5.8), as was discussed in [68]. Such a method was used for the simulations done in Paper G and Paper H.

5.2 Self-consistent simulations of mesoscopic devices

Transport in mesoscopic devices can, and has been studied using BPM (mainly by Palm et. al., see [67] and the papers upon which this is based). However if we are not interested in the dynamics of the device other time-independent methods may be more adequate depending on the problem at hand. The dominant approaches when it comes to simulation of transport in mesoscopic devices are mode-matching techniques [69, 70, 71, 72, 73] and methods based on Green’s functions [74, 75, 76, 77].

Commonly neglected in transport calculations is the contribution of the charge density distribution to the electrostatic potential as including this into the calculation considerably complicates the problem. The complication arises from the fact that to be able to calculate the charge density distribution, we need to know the potential. This in turn can be calculated if we know the charge density distribution, i.e. a computational catch 22. Since this is the case, the simulation has to be done self-consistently, meaning that we make an educated guess about the potential, calculate the charge density distribution from this, after which we calculate a new potential using the charge density distribution. Then we continue to iterate between calculations of a new potential and charge density distribution until
(hopefully) the difference between the calculated potential between two successive iterations is negligible. Obviously this can be very time-consuming which is why it is avoided whenever possible. It is however routinely used for e.g. calculations of electronic states in quantum wires and dots [78, 79].

To calculate the average charge density distribution $\rho$ of electrons in a mesoscopic device we need to know the wavefunction, $\psi$, since

$$\rho \propto |\psi|^2.$$  \hfill (5.10)

Mode-matching and Green’s functions methods do not yield the wavefunction explicitly and are thus not well suited for self-consistent simulations. It is thus preferable to use a method that is based on the calculation of the wavefunction directly. In Paper E a method, in which the wavefunction in the device is calculated using scattering states, was developed. For a general device such as that in Fig. 3.2 a scattering state $|j, k\rangle$ consists of a wave with wave-vector $k$ incident in lead $j$ together with scattered waves in all leads. It carries current from lead $j$ to lead $i$ as long as it is occupied [17]. The total charge density distribution in the device can be found by summing the contribution from the scattering states from all leads and then integrate over energy,

$$\rho(\vec{r}) = \frac{-e}{\pi} \int \sum_j f_j(k) |\psi_j(k)|^2 dk,$$ \hfill (5.11)

where $\psi_j(k)$ is the wavefunction in the device region of the scattering state $|j, k\rangle$. In doing so all electrons injected into the device are taken into account in the calculation of the charge density distribution, which is then coupled to a potential calculation self-consistently. This is a unique method as the charge density calculation distribution is energy-resolved and as such it is possible to accurately model mesoscopic devices with complex device geometries in which we expect the transmission probability matrix to be highly energy-dependent. It also makes it possible to consider devices to which a finite bias is applied where we cannot assume the transmission probability matrix to be constant over the energy-range in which transport occurs. The simulations done in Paper F were done using this method.

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\[1\] Nevertheless, Green’s functions have been used in such simulations [77].
Chapter 6

Fabrication of electron waveguide devices

Fabrication of semiconductor devices is a challenging task, but the abilities of modern semiconductor processing are, to say the least, impressive even for people working in the field. In this chapter we discuss how to actually achieve the confinement of electrons into the low-dimensional systems discussed in chapter 2 and how fabricate the electron waveguide devices of chapter 3.

6.1 From three dimensions to two

The confinement of electrons to two dimensions is achieved by the use of heterostructures. Basically this is a stack of different semiconductor materials (e.g. GaAs and AlGaAs) arranged in layers. Fabrication of heterostructures as such is a mature technology, which today is used in many commercial applications such as high-speed transistors and laser diodes. In 2000 Zhores I. Alferov and Herbert Kroemer were awarded the Nobel prize for the development of heterostructures\(^1\). The heterostructure used in Paper D was for instance from a HEMT (High Electron Mobility Transistor)-wafer bought from a commercial vendor.

Heterostructures are manufactured using epitaxy, and there are a number of different types of epitaxy. The basic principle is however to start with a substrate of a certain material (say InP) and then atomic layer by atomic layer are deposited, slowly growing the heterostructure. In Metal-Organic Vapor Phase Epitaxy (MOVPE) this is achieved by exposing the substrate to a reactive gas mixture, the gas reacts with the surface and deposits the desired atoms. By changing the composition of the gas we can then change what material is deposited. This can

\(^1\)Actually they shared half the prize, the other half went to Jack S. Kilby for his part in the invention of the integrated circuit
Chapter 6. Fabrication of electron waveguide devices

Figure 6.1. Confinement of electrons into one dimension by use of split-gates. Applying a negative potential to the gates on top of the structure will deplete the 2DEG below of electrons, thus confining electrons to the region in between the gates.

be controlled very precisely and it is thus possible to achieve transitions from one layer to another that are abrupt to the order of one atomic layer.

The fact that different semiconductor materials have different bandgaps can be used to confine electron to a very thin sheet if we arrange our different semiconductor layers properly. This as it is energetically favorable for the electrons to place themselves where they minimize their potential energy. This sheet can be formed either in a well, say a very thin layer (in the order of 15Å) of InGaAs sandwiched in between two layers of InP or just at an interface of two materials, for instance GaAs and AlGaAs. The sheet formed can be made sufficiently thin that the electrons will effectively be bound in the dimension that is perpendicular to the layers (the growth direction). Thus we have formed a two-dimensional system, a two-dimensional electron gas (2DEG).

As most basic semiconductor textbooks will tell you, semiconductors are in general poor conductors and to make them more conductive one adds doping atoms, which in essence are intentional impurities. These have loosely bound electrons that ionize easily, and it is these electrons that will form our 2DEG. By placing the dopants in a layer which is spatially separated from where the 2DEG is formed, a technique called modulation doping [80], the ions will not scatter the electrons as much as if they existed in the same plane (as they do in for instance a MOSFET). This means that the scattering rate of the electrons will decrease, increasing the mean free path. The ions can still scatter the electrons to a certain extent through a mechanism called remote-impurity scattering [81], although not as strong as impurity scattering, it can still cause strong variations in the potential distributions of individual electron waveguide devices [82].
6.2 From two dimensions to one

While the confinement of electrons to two dimensions as discussed above is a well established technology, confining them in yet another dimension is not. There are a number of techniques that have been demonstrated, each with its pros and cons.

A well-used technique that has delivered a large amount of interesting results is split-gate devices. In such devices lateral confinement is achieved by placing gates partially covering the top of the heterostructure and then applying a negative bias-voltage. This confines the electrons to the parts of the 2DEG where there is no gate on top, as seen in Fig. 6.1. The first demonstrations of quantized conductance were made in quantum point contacts (QPC) that were realized using split-gates [21, 22]. Split-gate devices have since been extensively used for investigations of electron transport phenomena. The first electron waveguide YBS was fabricated using the split-gate technology [84].

Split-gate devices have however one serious drawback for fabrication of electronic devices to that are to be used in practical applications rather than to be used for measuring and testing physical phenomena; the confining potential is rounded and and shallow. This means that the energy-difference between the confined modes is fairly small. If we consider fabricating single-mode devices we need a mode-spacing that is larger than temperature fluctuations, i.e. we need $\Delta E > k_B T$ (and preferably $\Delta E \gg k_B T$). If we require the device to function at room temperature or at least at elevated temperatures we thus need a large mode spacing. A more square-shaped potential like that of the example of a particle in a box in chapter 2 is what we want. Ideally we can achieve this if we etch away the heterostructure on both sides of the electron waveguide as in Fig. 6.2. In order to achieve side-walls that are vertical one can use a technique called reactive ion etching (RIE), in which
the heterostructure, after patterning is bombarded with ions that effectively ‘eats’ away the heterostructure which is not protected by the pattern (which can for instance be SiN). This is a high-energy technique which has the disadvantage of producing a lot of damage to the sidewall surface, with surface-states as a result. This makes the potential shape more smooth. A further consequence of the surface-states is that the electron waveguide defined will not be a straight channel; it will have a rather irregular channel-shape, producing surface scattering effects. In [83] quantized conductance in QPCs made using such a technique was demonstrated.

It is also possible to use wet chemical etching, in which the heterostructure is immersed into a suitable liquid etch-solution after patterning. Again, the parts of the heterostructure that is not covered by the pattern will be eaten away. This is a low-energy method and the amount of surface damage is lower than for dry etching (e.g. RIE). The drawback is however that a liquid etchant will generally etch with the same speed in all directions, the result of which is slanted walls as seen in Fig. 6.3. This reduces the degree of control of the geometry of the fabricated device.

6.3 Gates

The ability to control the electron device comes from the use of gates, and thus an important and integrated part of the device fabrication is the fabrication of these gates. As was discussed in 3.2, one of the main features of the YBS is that it theoretically is an extreme low-power switching device. The key point here is ‘theoretically’ as this is academic if we do not have effective gates. We do no only want to fabricate devices with gates, but devices with effective gates.

What then is an effective gate? Gating effectively means that we wish to change the electrochemical potential in the waveguide. Changing the electrochemical potential in an electron waveguide will change the number of populated sub-bands; the simplest way to get an estimate of the gate-efficiency is then to see how much you must change the gate-voltage in order populate one more sub-band. This will depend on screening of the gate-field, contact resistances and possibly other factors as well.

Defining the gating-efficiency in an electron waveguide is actually a bit more subtle since even for a perfect gate there is not a one-to-one correlation between the change in the electrostatic gate-voltage and the electrochemical potential in the waveguide, which is due to the low density of states in an electron waveguide, as is discussed in more detail in [87]. Also, the charge density in the electron waveguide will in itself screen the applied gate-field. In Paper F the self-consistent simulations indicated a gate-efficiency of 10% for switching in an YBS with idealized perfect gates.

The YBS discussed in [36] was defined by using RIE to deep-etch trenches. Gating was achieved by controlling the electrochemical potential in 2DEGs on the other side of the trenches. This scheme was originally proposed by Wieck and Ploog [85]
and is advantageous as it is a very simple fabrication method. Few process-steps are needed and the gates are automatically aligned. The cross-junction device in Paper C was also fabricate using this technique. On the other hand, the efficiency of the gates is low as the interfaces of the etched surfaces tend to screen the gate-potential [86]. By depositing Schottky-gates directly on the side walls of the electron waveguides it is possible to achieve more effective gates. The deposition can be done by means of an in-situ electrochemical process [88, 89]. The main advantage of this process is that before electrochemical deposition of the gates occur, the device is anodically etched in the same electrolyte. The transition from etching to plating is achieved simply by reversing the polarity of the electrode, and thus the device does not have to be removed from the electrolyte between etching and plating. The result can be oxide- and damage-free Schottky contacts. In Paper D YBSs were fabricated using this technique, and the characterizations done on these show a reduction in gate-voltage necessary to populate a new sub-band of the order of ten.

There are however drawbacks using this technique. First of all, the fabrication complexity is increased, three separate electron-beam lithography steps are required as opposed just one in the previous. The process works very well for GaAs/AlGaAs-devices but fabricating devices in using InGaAs/InP has proved very difficult with a yield for functioning gates that is extremely low (a few working InGaAs/InP devices have however shown positive results in term of improved gate-efficiency [90]). Schottky-diodes with good characteristics have been produced on planar InP-surfaces [91] but so far no stable technique for successful deposition of Schottky-type in-plane gates on etched InP/InGaAs devices have been reported. Another drawback of this device fabrication technique is that it employs wet-chemical etching as this gives good surface conditions for the electrochemical deposition of the gates. But as was discussed above, wet chemical etching reduces
the control of the geometry of the fabricated device as compared to dry etching and this generally leads to an YBS with a large branching region. This is undesirable as such an YBS may work more like a ballistic cavity coupled to three reservoirs via quantum point contacts rather than a coherent mode-evolution device. Ideally one would like to deposit Schottky-contacts on the side walls of waveguides defined by RIE, some preliminary experiments have been done, however due to the surface conditions caused by the dry etching, plating was very difficult to achieve [90].
Chapter 7

Summary and conclusions

In this chapter the articles on which this thesis is based are summarized, and the main conclusions stated. Additionally some general conclusions are drawn and some suggestions to extensions of the work are made. Where several authors cooperated, my contribution to the paper is stated.

7.1 Summary of the original work

**Paper A**: This paper analyzes interaction free measurements on quantum objects, two-level atoms, while most such treatments at the time considered classical objects. This is done in reference to a coupled atom-photon Mach-Zender interferometer and an atom-interferometer coupled with a cavity detector. The paper relates the classical interaction free measurements with quantum non-demolition measurements and discusses complementarity in such measurements.


**Paper B**: In response to the ‘phonon bottleneck’-discussion, this paper proposes a novel concept of carrier injection into low-dimensional lasers. The main point being that injecting electrons by means of an electron waveguide coupled to a quantum wire/box, the electrons could be injected *directly* into the exited state, circumventing time-consuming relaxation processes. The concept was studied on a quantum wire far IR laser. The paper is a proof-of-concept that by using coherent electron transport for carrier injection in low-dimensional lasers, injection directly into the exited state is possible.

*Contributions of the author of the thesis:* Development of concept together with co-authors, all computer simulations of the carrier injection as well as calculations of threshold current densities and modulation bandwidth of the quantum wire far IR laser.
Paper C: The transmission properties of a deep-etched electron waveguide cross-junction in InGaAs/InP-samples were measured at varying temperature and bias. As drift-diffusion transport theory predicts electrons to move between two neighboring arms and ballistic transport predicts electrons to go through the junction in a straight path, it was possible to study the transition between the two transport regimes. Partially ballistic transport was measured up to room temperature, which was the first demonstration of clear ballistic effects in deep-etched semiconductor structures at room temperature.

Contributions of the author of the thesis: Computer simulations of ballistic transport for the discussion of scattering in the different transport regimes.

Paper D: In order to achieve the theoretically promised low-power switching of the electron waveguide YBS highly effective gates are needed. Here electron waveguide YBSs were fabricated in GaAs/AlGaAs using a different kind of controlling gates than used for previously fabricated YBSs. The controlling gates were Pt/GaAs Schottky gates that were deposited on the devices by means of an \textit{in-situ} electrochemical process. Gate-efficiency was improved by a approximate factor of 10 as compared to previous in-plane gates.

Contributions of the author of the thesis: All device-design and fabrication. Characterization was done in collaboration with Katharina Hieke.

Paper E: In order to be able to more accurately model the transport in electron waveguide devices with complex geometries and to which a finite bias is applied, a new technique for self-consistent simulations was developed. The technique employs an energy-resolved calculation of the charge density distribution. The paper presents the computational technique, relates it with other simulation methods and presents some simulation examples. The computational technique should be applicable to a wide range of problems in the area of transport in mesoscopic devices, and as is discussed in the paper, there are a number of extensions possible.

Contributions of the author of the thesis: Development of the method in collaboration with Jan-Olof Wesström, all programming and simulations.

Paper F: The impact of space-charge on the ability to control the switching in an electron waveguide YBS was discussed. A previously proposed model to that end was evaluated and found inadequate. Self-consistent simulations of the switching behavior, using the method from Paper E, that supported the discussion were done. The simulations displayed a complex dependency of the switching on the space-charge, indicating that at lower charge densities the switching is as originally intended whereas at higher densities space-charge effects dominates.

Paper G: This paper is an attempt to assess the ultimate upper limit of the speed of electroabsorption modulators. The breakdown of the adiabatic approximation is discussed and the ultimate limit was put in relation to the response of the electron wavefunction to the modulating signal. The main conclusion was that, apart from
the obvious limit of the optical frequency itself, the theoretically attainable modulation rates are limited by the requirement of an adiabatic response of the electron wavefunction.

**Contributions of the author of the thesis:** Collaboration with the other authors on the assessments of the modulation limits as well as computer simulations of the wavefunction response.

**Paper H:** As a spin-off to the simulations in **Paper G** it was discovered that by using an asymmetrical quantum well it is possible to control the Rabi oscillations by means of an applied RF field. The concept is described and an analogy to coupled guided wave directional couplers is made. The conclusion was that a large number of states can be engineered artificially using the RF field.

**Contributions of the author of the thesis:** Development of concept in collaboration with Lars Thyén as well as all the simulations.

### 7.2 Some conclusions and the road ahead

Scientific work is in a sense never finished, new knowledge generates new questions and new ideas to explore. This is of course true for the work presented in this thesis and thus a brief discussion on possible extensions of this work is in order.

#### 7.2.1 Concerning the Y-branch switch

During the work on this thesis operating regimes other than the originally intended coherent switching regime have been discovered and pursued with great enthusiasm, see e.g. the discussion on ballistic switching in chapter 3.2. While highly interesting and encouraging results have been obtained one should however remember the key advantages of the coherent YBS, namely a power consumption not limited by the thermal energy. As the operating principle of the YBS in the ballistic switching regime is principally different than the coherent switching, power consumption that is not thermally limited by can not be expected. As low power consumption is the key in future nanoelectronics the coherent switching properties of the YBS remains its main advantage.

The effects of space-charge on the switching in the coherent regime are both substantial and complex as was discussed in **Paper F** and should prove to be an interesting field to probe further into. The results **Paper F** indicates that it is possible to operate the YBS in the coherent regime as originally intended if the total charge injected into the device remains low. Although this means that previously proposed Boolean logic gates based on the YBS could be operated as intended, it should be more beneficial to try to implement other kinds of logic using the YBS as a base device as discussed in chapter 3.2.2.

The main obstacle to low-power switching of coherent YBSs remains fabrication of effective gates. As shown in **Paper D**, required switching voltages of a YBS controlled by Pt/GaAs Schottky gates is significantly reduced as compared
to earlier gate-techniques, and the results indicates further room for improvement. However, as the deposition of the Schottky gates requires wet etching due to the surface conditions for plating, the degree of control of the device geometry is not satisfactory. The result is a comparably large ‘cavity’ in the branching region on the YBS. Multiple scattering in this cavity is probable with the possible loss of coherent transport as a result. Thus it can be said that further activities in coherent YBSs should focus on fabrication-issues, emphasizing the combination of large degree of geometrical control and high gate-efficiency.

### 7.2.2 Extending the self-consistent simulation tool

The simulation tool developed in Paper E has the possibility to become a very useful tool in mesoscopic device simulations and a number of extensions to the method, which are mentioned in the discussion at the end of the paper, can be considered. As presented in Paper E the algorithm only considers single-mode devices, which of course is a limitation, however extension to multi-mode devices is straight-forward. The same applies for extending the method to include magnetic fields.

The most interesting extension should however be the inclusion of a more realistic potential calculation. Ideally this would be done by including a full 3D Poisson equation with appropriate boundary conditions in the self-consistent iteration. Needless to say, this would be computationally very costly and the use of a parallel computer would be inevitable. The most time-consuming part of the algorithm is fortunately inherently parallel, and thus a very large and immediate gain could be achieved by doing this part in parallel without any further adaptations to parallel algorithms.

An intermediate step to achieve a more realistic potential calculation would be to calculate a realistic bare potential by a self-consistent 3D method as e.g. done in [35]. As the calculation of the bare potential is done only once in the setup of the simulation, the added computational time is small enough for this improvement to be done without porting the code to a parallel computer.

### 7.2.3 On the limit of modulation rates

The conclusions of Paper G discusses some upper limit to the possible modulation rates of intersubband electroabsorption modulators. The results are insightful, but it should be emphasized that the basic model is much simplified and as such the paper should be considered more the start of a debate than the final answer. Thus we can hope for more discussions on this matter, preferably concentrating on more realistic simulations.
Bibliography


[38] Attempts to verify the self-gating effect have been made both in our group and by L. Worschech et. al. at Würzburg University, see also discussions in: S. Retzenstein, L. Worschech, P. Hartmann, M. Kamp, and A. Forchel, *Capacitive-Coupling-Enhanced Switching Gain in an Electron Y-branch Switch*, Phys. Rev. Lett. **89**, 226804-1 (2002).


