Dissertation for the Degree of Doctor of Philosophy

# Signal propagation in open quantum wires 

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## Ågrip

Í ritgerðinni er notuð almenn stýrijafna án nálgunar Markovs til bess að lýsa tímahádum flutningi rafeinda um kerfi sem er skilgreint sem endanlegur fleygbogalagaður vír tengdur við tvær hálf-óendanlegar leið̊slur. Hægt er að prengja vírinn á einum eða tveimur stöðum. Endanlega skammtavírnum og leið̈slunum með̈ nokkrum orkuborðum er lýst með̈ samfellulíkani. Eiginástönd vírsins og leiðslanna eru reiknuð í ytra bverstæðu segulsviði. Tengingum leiðslanna og vírsins er lýst með óstað̊bundnum kjarna sem tengir bylgjuföll hvors kerfis ásamt pjálu tengifalli sem kveikt er á klukkan $\mathrm{t}=0$ til pess að rannsaka og ræða uppsöfnun hleðslu í vírnum, sveipstrauma um leiðslurnar og sístæða ástandið sem kerfið nálgast að lokum. Við kynnum hvernig tímaháðu tenginguna við vinstri leið̌sluna má nýta til að̃ vekja merki í vírnum sem nema má í hægri leiðslunni. Einnig er hægt að halda tengingunum við vinstri og hægri enda vírsins úr fasa til að líkja eftir skammtafæribandi. Forspennan sett á kerfið með̈ mismunandi efnamætti leið̊slanna, eiginleikar snertanna og áhrif tíðni á leiðnina eru bættir sem eru kannaðir með og án ytra segulsviðs. Við tökum eftir hvernig jaðarástönd sköpuð̛ af segulsviðinu taka pátt í dælingu rafhleðsslunnar um kerfið.


#### Abstract

In this thesis we use a non-Markovian generalized master equation to describe the time-dependent transport through a "sample system" defined as a parabolic quantum wire of a finite length coupled to two semi-infinite leads. The sample may also include one or two embedded quantum point contacts (QPCs). The quantum wire and the leads with several subbands are described by a continuous model. We calculate the eigenstates of the finite wire and of the leads in an external perpendicular magnetic field. The coupling between the leads and the sample are described by a non-local kernel connecting the wave functions from both sides and by a time-dependent coupling function with a smooth onset at the initial moment $t=0$ to investigate and discuss the charge accumulation in the sample, the transient currents along the leads, and the final steady state. We see how the time-dependent coupling of the left lead to the system can be used to generate a signal which is observed in the right lead. We can also keep the contacts out of phase to model a quantum turnstile. The chemical potential bias, the character of the contacts, the effects of the driving period, are examined in the absence and in the presence of the magnetic field. We observe how the edge states created in the presence of the magnetic field contribute to the pumped charge.


Always be ready to explain the fows and whys. George Santayana

## List of Papers

This thesis is based on the following papers

I Turnstile pumping through an open quantum wire Cosmin Mihai Gainar, Valeriu Moldoveanu, Andrei Manolescu, and Vidar Gudmundsson,
e-print arXiv:1004.4052, submitted for publication.

II Time-dependent magnetotransport in semiconductor nanostructures via the generalized master equation V. Gudmundsson, Chi-Shung Tang, Cosmin Mihai Gainar, Valeriu Moldoveanu, and Andrei Manolescu, Contribution to CCP-2009, Computer Physics Communications 182, (2010) 46-48.

III Time-dependent transport via the generalized master equation through a finite quantum wire with an embedded subsystem
V. Gudmundsson, C. Gainar, C. S. Tang, V. Moldoveanu, and A. Manolescu,
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## 1

## Introduction

Most electronic devices today use semiconductor components for processing electric signals. The study of semiconductor devices and the related technology is therefore an important branch of physics. These devices are modeled using quantum mechanics in order to take into account quantum effects in the restricted geometry. Low-dimensional devices are structures where the electrons can be confined in one or two dimensions in order to enhance the control of their density and conduction. When the electrons are confined in one spatial system dimension or on a long two-dimensional strip they create a quantum wire. A quantum wire is an electrically conducting system, in which quantum effects are affecting transport properties. The electrons can also be confined in all directions resulting in a quantum dot.

Quantum wires and dots are created from a two-dimensional electron gas (2DEG) by using lateral confinement potentials in the plane of the 2DEG produced by metal electrodes at some distance from the 2DEG.

A two-dimensional electron gas of high mobility can be formed at an interface of AlGaAs and GaAs in a semiconductor. The reason why these semiconductors are chosen is that they have a similar lattice constant (GaAs - 5.653A and AlGaAs - 5.660A) while the energy gaps between

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the conduction and valence band differ. Using the technique of Molecular Beam Epitaxy (MBE), they are grown on top of each other, with atomic monolayer precision (see Figure 1.1).


Figure 1.1: GaAs/AlGaAs:Si heterostructure used to make a 2DEG.

A layer of GaAs is grown on a substrate, usually made of GaAs. Then a layer of undoped AlGaAs followed by a layer of Si doped AlGaAs. The Si atoms act as donors for the 2DEG and the undoped layer acts as a barrier between the electrons and the donors to minimize electron scattering by the ionized donors. On top of this another GaAs layer is grown, called cap layer which keeps the Al from oxidizing. At very low temperatures, 3D semiconductors are insulating but in 2D system or a quantum wire there can be a metallic type electronic system. By doping the AlGaAs-layer with Si-donors, free carriers are introduced (the conduction electrons move to the GaAs-layer). A triangular potential is formed at the interface and the conduction electrons are confined by this potential to a layer of thickness $\approx 10 \mathrm{~nm}$, leading to a quantization of the electron motion perpendicular to the interface and a free motion in
the $x-y$ plane parallel to the AlGaAs/GaAs interface. The energy levels have the following form

$$
\begin{equation*}
E=E_{a}+\frac{\hbar}{2 m^{*}}\left(k_{x}^{2}+k_{y}^{2}\right) . \tag{1.1}
\end{equation*}
$$

In the above equation $m^{*}$ is the effective mass of the electron, $k_{x}$ and $k_{y}$ are the wave-vectors in the plane of the 2DEG and $E_{a}$ are the electric quantum levels arising from the confinement in the growth direction. The effective Bohr radius in GaAs is $a_{0}^{*}=9.79 \mathrm{~nm}$. In this approximation the effect of the surrounding lattice is included in the effective mass ( $m^{*}=0.067 m_{e}$ for GaAs, and $m_{e}$ is the free-electron mass). The static transport properties of low dimensional systems of this type have been intensively studied since about 1980, both theoretically and experimentally.

More recently, the time-dependent properties of semiconductor nanostructures and their response to electric pulses become accessible through transient current measurements and in a pump-and-probe configuration (1;2;3). With these experimental developments theoretical schemes for the description of time-dependent transport emerged. The methods include the non-equilibrium Keldysh-Green function formalism (4; 5), Lippmann-Schwinger formalism (6), and more recently the generalized master equation (GME) adapted for electronic transport (7; 8). The non-equilibrium Keldysh-Green function formalism is a useful tool for first-principles studies of non-equilibrium many-particle systems.

Caroli et al. (9), applied the Keldysh formalism to mesoscopic transport. Starting from a very simple model Hamiltonian they considered that a description of the system as a whole does not permit the calculation of the current, because tunneling is a non-equilibrium process. This is one of the reasons for using an effective Hamiltonian of type: $H_{\text {eff }}=H_{L}+H_{R}+T$; with $H_{L}$ and $H_{R}$ corresponding to two disconnected systems. $T$ is the transfer term which induces transitions of an

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electron between these two systems. The transition probability is calculated by means of first order time dependent perturbation theory.
They realized that the current can be calculated directly, even at finite voltage, with the help of the theory of perturbations in non-equilibrium systems. Within this framework it is also possible to take into account many-body effects systematically, without any of the difficulties encountered in the usual tunneling formalism.

Recently, Moldoveanu et al. (10) calculated transient currents from the non-equilibrium Green-Keldysh formalism for a many-level finite system coupled to semiinfinite biased leads. Here, the numerical simulations are restricted to the steplike coupling of the sample to the leads. The model allows consideration of more general time-dependent potentials between the leads and the central region or sample.
In contrast to most of the previous studies they describe a time dependent current through systems with more complex structure than only one ore two levels. By increasing the system size the shape of the transient current and the evolution towards the steady state differs significantly from the single-site oscillatory behavior and depends crucially on the number of electronic states available in the bias window.
The electron-electron interaction plays an important role in the transient behavior and the formalism allows the inclusion of Coulomb terms in the Hamiltonian, but they did not take it into account because the Coulomb interaction in the Keldysh approach is very complex and requires strong approximation schemes for the self-energy.

Another method used to describe the conductivity of open systems is the Lippmann-Schwinger scattering approach. Thorgilsson et al. (11) demonstrated and elucidated how the embedded quantum dots in a uniform perpendicular magnetic field affect the transport characteristics of the electron wave packet in a quantum wire system. By changing the embedded potential and the scattering wave function into a momentumcoordinate representation, they found that the wave packet transmission
probability can be obtained using the Lippmann-Schwinger method extended to the time-domain. They considered embedded antidot and double-dot systems in an external magnetic field.

The Lippmann-Schwinger formalism and the non-equilibrium Green functions methods have been used for predicting $I / V$ characteristics of quantum systems connected to two metal leads. The point is that both theories are exact in their respective domains: LS is limited to elastic processes while the NEGF can treat both elastic and inelastic processes.

The quantum master equation approach is an alternative tool for studying the irreversible dynamics of quantum systems coupled to a macroscopic environment. Owing to its simple structure, it provides an intuitive understanding of the system dynamics and has been used in various fields such as quantum optics (12; 13), solid state physics (14) and chemical dynamics (15).

The natural theoretical tool for investigating transitions and computing life times is the reduced density operator (RDO) method which gives information about the sample in the presence of the leads. The general strategy goes as follows: 1) One starts with disconnected subsystems, i.e. a sample $S$ and some particle reservoirs characterized by different chemical potentials; 2) at an initial instant the sample is coupled to the reservoirs via a transfer Hamiltonian $H_{T}$ which is time-dependent; 3) starting from the quantum Liouville equation for the statistical operator $W(t)$ that describes the total system one performs a partial trace over the reservoirs and writes down an integro-differential equation for the reduced density operator (RDO). This equation is called the generalized Master equation because it contains both diagonal and off-diagonal elements of RDO. The effect of the reservoirs on the sample is taken into account through the so-called memory kernel which contains an infinite sum of time-ordered multiple commutators of the type $\left[H_{T},\left[. .\left[H_{T}, \rho\right]\right]\right.$. Otherwise stated, in its general form the equation for the RDO is nonMarkovian. Usually the effect of the leads is taken into account up

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to the second order in $H_{T}$, in the kernel of the integro-differential equation, which at the physical level describes sequential tunneling processes. There are several versions of the GME method that have been proposed in the context of quantum transport.

Harbola et al. (16) used the GME to calculate the dynamics of a quantum system connected to two leads with different chemical potentials using projection operators which project the total many-body density matrix of the system into the system subspace corresponding to a fixed number of electrons. Studying the transient and steady-state transport properties of a coupled quantum dot the authors found that coherence between the many-body levels can affect the transport properties of the quantum system.

Gurvitz and Prager (17) were the first to derive a hierarchy of QMEs which keeps track of the number of electrons transferred from the source lead to the collector lead. Using this hierarchy they studied the effects of quantum coherence and Coulomb blockade in steady-state electron transport in the high bias limit.

Moldoveanu et al. (18) solved the GME using the Crank-Nicolson algorithm for the time integration. The numerical simulations were performed for a lattice Hamiltonian. They computed the transients properties associated with each level of a 2D lattice in the presence of a strong perpendicular magnetic field. The authors presented the analysis of the electron dynamics in the transient regime and also studied the matrix elements (population and coherence) of the reduced density operator.

The Coulomb interaction inside the sample was not included in this work but in another paper (19) they combined the GME method with the Coulomb interaction. Using three sample models, a short 1D wire with five sites, but also a larger 2D lattice with 120 sites and a continuous model (20) they analyzed the dynamics of the electrons starting with the moment when the leads are coupled to the sample until a steady state is reached. Because the Fock space increases exponentially with the number
of SES it is possible to describe just few electrons in the system (they have up to 12 SESs in a reduced Fock space). These studies were very important for understanding the transient regime and the steady-state.

Other important aspects in the time-dependent transport calculations are quantum pumping and turnstile pumping. A pump is a device that generates a DC current due to an oscillating input. In the simplest configuration a pump has two leads connected to two reservoirs. The pump takes particles from one reservoir and transfers them into the other. A current is produced even if the reservoirs have the same temperature and chemical potential.

There are experimental realizations of electron pumps in semiconductor quantum dots using the principle of Coulomb blockade. If the dot is coupled to the outside world via tunneling point contacts, the charge on the dot is quantized and transport is inhibited for certain ranges in the bias as a result of the high energy cost of adding an extra electron to the dot.

The first experiment on electron pumping in single electron devices was performed by Pothier et al. (21). They constructed an electron pump operating at low frequency and with a reversible pumping direction. The pump consists of three tunnel junctions in the Coulomb blockade regime and works through a mechanism that closely resembles a peristaltic pump: charge is pumped through the junctions from the left to the right, electron-by-electron as the voltage $U_{1} \propto \sin (\omega t)$ of the left dot reaches its minima and maxima before the voltage $U_{2} \propto \sin (\omega t-\phi)$ of the right one. The pumping direction can be reversed by reversing the phase difference $\phi$ of the two gate voltages.

Adiabatic quantum pumping in mesoscopic noninteracting open quantum dots was investigated theoretically by Brouwer (22) by means of a scattering approach. He demonstrated that the pumping current is proportional to the driving frequency and shows large mesoscopic fluctuations.

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Torres (23), studied quantum charge pumping in a system with a single time-periodic parameter where the pump consists of a ring connected to two leads and containing a subsystem embedded in one of its arms. He showed that a pumped current proportional to the square of the driving frequency appears as a result of the combined effect of spatial interference through the ring and photon-assisted tunneling.

In another paper, Cota et al. (24), proposed and analyzed a new scheme of realizing both spin filtering and spin pumping by using a double quantum dot, with the time-dependent gate voltages in the presence of a magnetic field including electron-electron interaction. The results demonstrated that the width in frequency of the spin-up pumped current gives information about spin decoherence in the quantum dot.

On the another hand, a turnstile pump is a single-electron device where the sample is periodically connected and disconnected with the left and right lead respectively, but with a relative phase shift. This setup is different from a quantum pump where a current is generated by asymmetric external oscillations, but without a bias. It was experimentally created by Kouwenhoven et al. (25) by modulating in time the two tunneling barriers between a quantum dot and two leads. The electrons were driven by a finite bias between the leads.

In a recent publication, Moldoveanu et al. (26) investigated the modulation of the drain current when a sequence of square pulses is applied to the source probe connected to a quantum dot and a short quantum wire described within lattice model. This model set-up is close to the experiments by Naser et al. and Lai et al. A characteristic of this kind of experiments is that the chemical potentials of the leads are such that the first excited state is above the bias window, while the ground state is embedded in it. Obviously, the current in the leads cannot capture all the details of the dynamics of electrons in the sample.

Considering all of these, the aim of this thesis is to investigate the time-dependent transport in mesoscopic structures by solving the GME
without using the Markov approximation and we propose an implementation of the generalized master equation which allows us to take into account the geometry of the sample. The results are obtained using a pure finite quantum wire with parabolic confinement and a wire with an embedded constriction (a potential barrier). The quantum wire considered has a complex structure. We start from the single-particle Hamiltonian of a two-dimensional wire of length $L_{x}$ parabolically confined along the $y$ direction and with hard-wall conditions at $\pm L_{x} / 2$. We put a special effort on describing the lead-sample contacts which are opened and closed periodically by simulating rectangular pulses on metallic strip gates which define the contact region. The calculations can be performed, both in the absence and in the presence of the magnetic field.

1. INTRODUCTION

## 2

## Description of the central system

In this chapter we analyze a physical system which consists of two elements: $\mathcal{A}$, a finite quantum wire and $\mathcal{B}$, two semi-infinite leads. The system is depicted on Figure 2.1. We are interested in what happens in $\mathcal{A}$ which is much smaller than part $\mathcal{B}$. Subsystem $\mathcal{B}$ is important for the injection (extraction) of electrons in subsystem $\mathcal{A}$, and the $\mathcal{A}-\mathcal{B}$ interaction affects the evolution of $\mathcal{A}$. Actually, $\mathcal{B}$ is a reservoir (27; 28), and plays the role of an environment which is defined by external factors. All of this is important in the context of quantum information theory (29;30), when the relevant subsystem is influenced by the surroundings.


Figure 2.1: A schematic view of the sample to the leads.

## 2. DESCRIPTION OF THE CENTRAL SYSTEM

### 2.1 Finite isolated quantum wire in magnetic field

The electronic states in an infinitely long wire with parabolic lateral confinement or lateral hard walls can be calculated analytically. This is no longer possible if the wire is finite in length and in a constant magnetic field, perpendicular to the wire. This kind of system can not be solved analytically but we can find the eigenvalues and eigenvectors of the corresponding Hamiltonian numerically.

We consider an isolated finite quantum wire, extended in the $x$ direction. The width of the wire is defined by a parabolic confinement potential in the $y$-direction with the characteristic energy $\hbar \Omega_{0}=1.0$ meV . The quantum wire is terminated at $\pm L_{x} / 2$ with hard wall potentials as shown in Figure 2.2. This is the subsystem $\mathcal{A}$, which we will also call the "sample".


Figure 2.2: A finite length wire in a constant magnetic field.
The Hamiltonian of the sample in a magnetic field is defined as follows

$$
\begin{equation*}
H_{S}=H_{0}+V_{\text {conf }}(y) \tag{2.1}
\end{equation*}
$$

where $H_{0}$ describes a particle moving in two dimensions under the action of a constant magnetic field and $V_{\text {conf }}(y)$ is the lateral confinement
potential.

### 2.1.1 Confinement potential

To describe the confinement potential we use a harmonic oscillator potential

$$
\begin{equation*}
V_{\text {conf }}(y)=\frac{1}{2} m^{*} \Omega_{0}^{2} y^{2} \tag{2.2}
\end{equation*}
$$

This confinement in vanishing external magnetic field gives "rise" to eigenstates $\psi_{a}^{S}(x, y)$ that are solutions to the eigenvalue equation, $(a$ indicates a quantum number of the system)

$$
\begin{equation*}
\left[-\frac{\hbar^{2}}{2 m^{*}}\left(\frac{d^{2}}{d x^{2}}+\frac{d^{2}}{d y^{2}}\right)+V_{c o n f}(y)\right] \psi_{a}^{S}(x, y)=E_{a} \psi_{a}^{S}(x, y) \tag{2.3}
\end{equation*}
$$

where $E_{a}$ are the eigenvalues of $H_{S}$.
In the presence of a magnetic field oriented along the $z$ direction, $\mathbf{B}(\mathbf{r})=B \mathbf{e}_{\mathbf{z}}$, we chose the vector potential in the Landau gauge, $\mathbf{A}(\mathbf{r})$ $=(-B y, 0,0)$, and obtain

$$
\begin{equation*}
H_{S}=\frac{1}{2 m^{*}}\left[\left(p_{x}-\frac{e}{c} B y\right)^{2}+p_{y}^{2}+\Omega_{0}^{2} y^{2}\right] . \tag{2.4}
\end{equation*}
$$

A more convenient form of $H_{S}$ can be obtained with the help of the following notations

$$
\begin{align*}
\Omega_{w}^{2} & =\Omega_{0}^{2}+\Omega_{c}^{2} & \Omega_{c}^{2} & =\left(\frac{e B}{m^{*} c}\right)^{2} \\
l^{2} & =\frac{\hbar c}{e B}=\frac{\hbar c}{m^{*} \Omega_{c}} & a_{w} & =\sqrt{\frac{\hbar}{m^{*} \Omega w}} \tag{2.5}
\end{align*}
$$

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where the constant $l$ is called the magnetic length and $a_{w}$ has the dimension of length. Then we can write

$$
\begin{equation*}
H_{S}=\underbrace{\frac{1}{2 m^{*}} p_{x}^{2}}_{H_{x}}+\underbrace{\left[\frac{1}{2 m^{*}} p_{y}^{2}+\frac{1}{2} m^{*} \Omega_{w}^{2} y^{2}\right]}_{H_{y}}+\underbrace{\frac{\hbar c}{m^{*} l^{2}} p_{x} y}_{H_{x, y}} \tag{2.6}
\end{equation*}
$$

In fact, our system consists of an infinite potential well in the $x$ direction, a harmonic oscillator with frequency $\Omega_{\omega}$ in the $y$ direction and a coupling in the $x$ and $y$ direction proportional to $p_{x} y$.

We write the eigenstates of the Hamiltonian $\left.H_{S}, \mid \alpha\right)$, as a linear combination of the vectors in the complete orthonormal basis $|\alpha\rangle$ consisting of the eigenstates of the Hamiltonian $H_{x}+H_{y}$, i.e. the product of the eigenstates of $H_{x}$ and the eigenstates $H_{y},|\alpha\rangle=\left|n_{x} n_{y}\right\rangle$. Thus

$$
\begin{equation*}
|\alpha\rangle=\sum_{\beta}|\beta\rangle\langle\beta \mid \alpha\rangle=\sum_{\beta} C_{\beta \alpha}|\beta\rangle . \tag{2.7}
\end{equation*}
$$

The eigenvalue equation

$$
\begin{equation*}
\left.\left.H_{S} \mid \alpha\right)=\epsilon_{\alpha} \mid \alpha\right) \tag{2.8}
\end{equation*}
$$

is then solved by projecting it on the $|\beta\rangle$-basis and using the expansion (2.7) for the eigenstates $\mid \alpha$ ) resulting in

$$
\begin{equation*}
\sum_{\gamma} C_{\gamma \alpha}\left\{E_{\gamma} \delta_{\beta \gamma}+\langle\beta| H_{x y}|\gamma\rangle\right\}=\epsilon_{\alpha} C_{\beta \alpha} \tag{2.9}
\end{equation*}
$$

We know that without $H_{x y}$ the problem is separable

$$
\begin{equation*}
E_{n_{x} n_{y}}=E_{n_{x}}^{x}+E_{n_{y}}^{y} \tag{2.10}
\end{equation*}
$$

$H_{x}$ is the Hamiltonian for an infinite square well, and thus

$$
\begin{equation*}
E_{n_{x}}^{x}=\hbar \Omega_{\omega} \frac{a_{\omega}^{2}}{L_{x}^{2}} \frac{n_{x}^{2} \pi^{2}}{2} \tag{2.11}
\end{equation*}
$$

$H_{y}$ is the Hamiltonian for an harmonic oscillator, so

$$
\begin{equation*}
E_{n_{y}}^{y}=\left(n_{y}+\frac{1}{2}\right) \hbar \Omega_{\omega}, \quad n_{y}=0,1,2, \ldots, \tag{2.12}
\end{equation*}
$$

Combining these, we have

$$
\begin{equation*}
E_{n_{x} n_{y}}=\hbar \Omega_{\omega}\left[n_{y}+\frac{1}{2}+\frac{a_{\omega}^{2}}{L_{x}^{2}} \frac{n_{x}^{2} \pi^{2}}{2}\right] \tag{2.13}
\end{equation*}
$$

The energy spectrum $\epsilon_{\alpha}$ and the states $\left.\mid \alpha\right)$ are found by diagonalizing the set of coupled linear eigenvalue equation (2.9) afther the matrix elements of $H_{x y}$ are evaluated analytically.

### 2.1.2 Embedded subsystem

To study the effects of the geometry of the sample we include an embedded subsystem. The new Hamiltonian of the sample becomes

$$
\begin{equation*}
H_{S} \rightarrow H_{S}+W(x, y) \tag{2.14}
\end{equation*}
$$

with $W(x, y)$ a combination of Gaussian potentials. It is sufficient for us to show the method of solution for one such potential

$$
\begin{equation*}
W(x, y)=V e^{\left[-\beta_{x, 1}\left(x-x_{1}\right)\right]^{2}-\left[\beta_{y, 1}\left(y-y_{1}\right)\right]^{2}} \tag{2.15}
\end{equation*}
$$

where $V$ is the strength of the potential, while $\left(x_{1}, y_{1}\right)$ and $\beta_{(x, y), 1}$ control the location and the range of the potential. In Figure 2.3(a,b), for

## 2. DESCRIPTION OF THE CENTRAL SYSTEM

the positive potential ( $V=3 \mathrm{meV}$ ) we would expect to see an antidot and respectively a dot if the potential is negative $(V=-3 \mathrm{meV})$.
On the other hand, by varying the parameters $x_{1}, y_{1}$, we have the possibility to change the placement of the Gauss potential as shown in Figure $2.3(\mathrm{c}, \mathrm{d})$ for $x_{1}=250 \mathrm{~nm}$ and $y_{1}=20 \mathrm{~nm}$.
The matrix elements of $W(x, y)$ are evaluated in appendix A.2.


Figure 2.3: The potential of a quantum wire with an embedded subsystem. $L_{x}=900 \mathrm{~nm}$.

### 2.1.3 Properties of eigenstates

## Pure finite quantum wire in vanishing external magnetic field

Before describing the transport formalism for the system we need to investigate the equilibrium properties of the disconnected subsystems, the semi-infinite leads and the finite quantum wire.

The eigenvalues of the system are shown in Figure 2.4.


Figure 2.4: The energy spectrum of the pure isolated quantum wire for vanishing external magnetic field. $L_{x}=900 \mathrm{~nm}$. The horizontal axis $a$ shows the index of the state in an increasing energy order.

The position of the arrows indicates the eigenstates for which we plot the probability density in Figure 2.5. In the lowest part of the energy spectrum one can distinguish subband created by the oscillator states. The states 1,2 and 4, are situated in the lowest subband and the state 5 in the next subband; therefore the probability densities for the states 1,2 and 4 , have one maxima in the $y$ direction, while the probability density for the state 5 has two maxima.

## Constant external magnetic field

In Figure 2.6 we plotted the energy spectra of the pure wire without and with magnetic field. For $a=1$ we see how the magnetic field has very little effect compared to the previous case. By increasing the energy, for $a=8$, we obtain an edge state. For $a=12$, we have a similar situation as before for $a=5$ : the probability is concentrated in the bulk of the wire and with a split maximum.

Constant magnetic field and embedded potential well-or hill
As we would expect, a potential well described by a Gauss potential reduces the energy values while the positive Gauss potential raises them.


Figure 2.5: The probability density of the single-electron eigenstates of the pure wire for vanishing external magnetic field. $L_{x}=900 \mathrm{~nm}$.


Figure 2.6: The energy spectrum of the pure wire for $B=1 \mathrm{~T}$ in comparison with $B=0$ T. $L_{x}=900 \mathrm{~nm}$.


Figure 2.7: The probability density of the single-electron eigenstates of the pure wire for $B=1 \mathrm{~T} . L_{x}=900 \mathrm{~nm}$.


Figure 2.8: The energy spectra of the finite quantum wire with an embedded Gaussian well for $B=1 \mathrm{~T}$ and $V= \pm 3 \mathrm{meV} . L_{x}=900 \mathrm{~nm}$.

## 2. DESCRIPTION OF THE CENTRAL SYSTEM

This is shown in Figure 2.8.
We note that the energy of the 1st state is negative for $V=-3 \mathrm{meV}$. In Figure 2.9 we remark that for $a=1$, the negative potential traps the electron, while a positive potential splits the electron localization in two distinct peaks. For $a=3$, for a negative potential, the electron is drawn to the center, but in the last case $(V=3 \mathrm{meV})$, two distinct circular orbits are created.


Figure 2.9: The probability density of the single-electron eigenstates of the finite quantum wire with an embedded well (left) or hill (right) for $B=1 \mathrm{~T}$ and $V= \pm 3 \mathrm{meV} . L_{x}=900 \mathrm{~nm}$.

## 3

## Generalized Master Equation formalism

### 3.1 Coupled system

In this section we introduce the Hamiltonian of the total system consisting of the leads and the sample. To make the connection between the sample and the leads we define a transfer Hamiltonian. Such a transfer Hamiltonian was introduced in the early days of electronic quantum transport and discussed in a series of papers (31; 32; 33). The transfer Hamiltonian has also been used within the non-equilibrium GreenKeldysh transport formalism. Usually the wide-band limit approximation was assumed and the energy dependence of the coupling coefficients was neglected (34).

### 3.1.1 Modeling the contacts

We consider three subsystems: the two semi-infinite leads $l=L, R$ (left and right), and the central sample which is a finite two dimensional wire in $x y$-plane. In the $y$-direction the electrons in the sample are parabolically confined with the characteristic energy $\hbar \Omega_{0}$, but in the $x$-direction

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they are confined by hard walls at $x= \pm L_{x} / 2$. The effective width of our typical sample is about $4-5$ times smaller than the length.
We denote by $\psi_{a}^{S}(\mathbf{r})$ and $E_{a}$ the eigenfunctions and eigenvalues of the single-particle Hamiltonian $H_{S}$ where $a$ indicates the two quantum numbers of the system, $n_{x}^{S}$ and $n_{y}^{S}$. The reservoirs have different chemical potentials. The single-electron Hamiltonian of the left and the right leads is noted by $H_{L}$ or $H_{R}$, respectively. Their eigenfunctions are $\psi_{q}^{L, R}(\mathbf{r})$ and the eigenvalues are $\epsilon^{L, R}(q)$, where $q$ stands both for a continuous wave number and a discrete subband number $n_{y}^{L, R}$ defined by the parabolic confinement in the $y$ direction.

The single particle Hamiltonian of the disconnected system is

$$
\begin{equation*}
H_{0}=H_{L}+H_{R}+H_{S} \tag{3.1}
\end{equation*}
$$

where $H_{S}$ is

$$
\begin{equation*}
H_{S}=\frac{\mathbf{p}^{2}}{2 m^{*}}+\frac{1}{2} m^{*} \Omega_{0}^{2} y^{2}+W(\mathbf{r}) \tag{3.2}
\end{equation*}
$$

with $W(\mathbf{r})$ representing an embedded subsystem in the wire.
Our method can be implemented both for continuous or discrete models. Here we shall present only the continuous case.

Using the eigenstates corresponding to the isolated sample and leads we write the Hamiltonians of the disconnected subsystems as

$$
\begin{equation*}
H_{S}=\sum_{a} E_{a}\left|\psi_{a}^{S}\right\rangle\left\langle\psi_{a}^{S}\right|, H_{L, R}=\sum_{q} \epsilon^{L, R}(q)\left|\psi_{q}^{l}\right\rangle\left\langle\psi_{q}^{l}\right| \tag{3.3}
\end{equation*}
$$

In order to describe the coupling between the two subsystems we add a perturbation to $H_{0}$. The single-particle form of the transfer Hamiltonian can be written as

$$
\begin{equation*}
H_{T}(t)=\sum_{l=L, R} \sum_{a} \sum_{q} \chi_{l}(t)\left(T_{q a}^{l}\left|\psi_{a}^{S}\right\rangle\left\langle\psi_{q}^{l}\right|+h . c\right) . \tag{3.4}
\end{equation*}
$$

The time-dependent part of the coupling is controlled by the switching functions $\chi_{l}(t)$, with $l=L, R$. At $t=t_{0}$ the sample and the leads are disconnected, i.e. $\quad \chi_{l}\left(t=t_{0}\right)=0$, and they are gradually coupled for $t>t_{0}$, i.e. $\chi_{l}\left(t>t_{0}\right)>0$, and $\chi_{l}(t \rightarrow \infty)=1$, if we wish to keep the subsystem coupled ever after.

Now, because we have an open system with variable number of particles (recall that the semi-infinite leads simulate particle reservoirs) it is natural to use a many-particle Hamiltonian, although we shall completely neglect the Coulomb interaction for the electrons in the central system and the leads. The many-body formalism allows us to account for electron correlations in the central system imposed on it by the coupling to the leads. According to the general rules of second quantization (35) a basis in the Fock space $\mathcal{F}$ of the coupled system can be constructed starting from the eigenfunctions $\psi_{a}^{S}(x, y)$ and $\psi_{q}^{L, R}(x, y)$. One defines creation and destruction operators for electrons in the leads $c_{q l}^{\dagger}\left(c_{q l}\right)$ and in the sample $d_{a}^{\dagger}\left(d_{a}\right)$. Then the second-quantized total Hamiltonian reads as follows

$$
\begin{equation*}
H(t)=\sum_{a} E_{a} d_{a}^{\dagger} d_{a}+\sum_{q, l=L, R} \epsilon^{l}(q) c_{q l}^{\dagger} c_{q l}+H_{T}(t) \tag{3.5}
\end{equation*}
$$

where the tunneling Hamiltonian $H_{T}(t)=H_{T}^{L}(t)+H_{T}^{R}(t)$ describes the coupling of the system to the left and right leads

$$
\begin{equation*}
H_{T}^{l}(t)=\chi_{l}(t) \sum_{q, a}\left\{T_{q a}^{l} c_{q l}^{\dagger} d_{a}+\left(T_{q a}^{l}\right)^{*} d_{a}^{\dagger} c_{q l}\right\} \tag{3.6}
\end{equation*}
$$

The coefficients $T_{q a}^{l}$ following from Equation (3.3) could have the form

$$
\begin{equation*}
T_{q a}^{l} \sim\left[\psi_{q}^{l}\left( \pm L_{x} / 2\right)\right]^{*}\left[\psi_{a}^{S}\left( \pm L_{x} / 2\right)\right] \tag{3.7}
\end{equation*}
$$

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Rigorously speaking the states in the isolated sample and leads vanish at the boundaries $\pm L_{x} / 2$, such that according to the definition (3.7), $T_{q a}^{l}=0$.
Therefore we shall adopt a phenomenological assumption (ansatz) that the transfer coefficients are in fact given by a non-local overlap of a pair of eigenstates $\left(\psi_{a}^{S}, \psi_{q}^{l}\right)$ on a domain $\Omega_{S}^{l} \times \Omega_{l}$ defining the contact between the sample and the $l$-th lead. The coupling strength tensor $T_{q a}^{l}$ is thus modeled as

$$
\begin{equation*}
T_{q a}^{l}=\int_{\Omega_{S}^{l} \times \Omega_{l}} d \mathbf{r} d \mathbf{r}^{\prime}\left(\psi_{q}^{l}\left(\mathbf{r}^{\prime}\right)\right)^{*} \psi_{a}^{S}(\mathbf{r}) g_{a q}^{l}\left(\mathbf{r}, \mathbf{r}^{\prime}\right)+h . c . \tag{3.8}
\end{equation*}
$$

We chose the integration domains for the leads as

$$
\begin{align*}
& \Omega_{L}=\left\{(x, y) \left\lvert\,\left[-\frac{L_{x}}{2}-2 a_{w},-\frac{L_{x}}{2}\right] \times\left[-3 a_{w},+3 a_{w}\right]\right.\right\} \\
& \Omega_{R}=\left\{(x, y) \left\lvert\,\left[+\frac{L_{x}}{2},+\frac{L_{x}}{2}+2 a_{w}\right] \times\left[-3 a_{w},+3 a_{w}\right]\right.\right\} \tag{3.9}
\end{align*}
$$

and for the sample

$$
\begin{align*}
\Omega_{S}^{L} & =\left\{(x, y) \left\lvert\,\left[-\frac{L_{x}}{2},-\frac{L_{x}}{2}+2 a_{w}\right] \times\left[-3 a_{w},+3 a_{w}\right]\right.\right\} \\
\Omega_{S}^{R} & =\left\{(x, y) \left\lvert\,\left[+\frac{L_{x}}{2}-2 a_{w},+\frac{L_{x}}{2}\right] \times\left[-3 a_{w},+3 a_{w}\right]\right.\right\} \tag{3.10}
\end{align*}
$$

In Equation (3.8) the function

$$
\begin{equation*}
g_{a q}^{l}\left(\mathbf{r}, \mathbf{r}^{\prime}\right)=g_{0}^{l} \exp \left[-\delta_{1}^{l}\left(x-x^{\prime}\right)^{2}-\delta_{2}^{l}\left(y-y^{\prime}\right)^{2}\right] \exp \left(\frac{-\left|E_{a}-\epsilon^{l}(q)\right|}{\Delta_{E}^{l}}\right) \tag{3.11}
\end{equation*}
$$

with $\mathbf{r} \in \Omega_{S}^{l}$ and $\mathbf{r}^{\prime} \in \Omega_{l}$ defines the coupling of any two single-electron states by the 'nonlocal overlap' of their wave functions in the contact region of the leads and the sample. The parameters $\delta_{1}^{l}$ and $\delta_{2}^{l}$ define the spatial range of the coupling within the chosen domains $\Omega_{S}^{l} \times \Omega_{l}$.

### 3.1.2 Reduced Density Operator

After introducing the second quantized Hamiltonian $H(t)$ we now define the statistical operator of the whole quantum system as the solution of the Liouville equation

$$
\begin{equation*}
i \hbar \dot{W}(t)=[H(t), W(t)], \quad W\left(t<t_{0}\right)=\rho_{L} \rho_{R} \rho_{S} \tag{3.12}
\end{equation*}
$$

where $\rho_{S}$ is the density operator of the isolated sample (at $t<t_{0}$ ) and $\rho_{L, R}$ are the density operators of the disconnected lead $l=L, R$

$$
\begin{equation*}
\rho_{l}=\frac{e^{-\frac{1}{k T}\left(H_{l}-\mu_{l} N_{l}\right)}}{\operatorname{Tr}_{l}\left\{e^{-\frac{1}{k T}\left(H_{l}-\mu_{l} N_{l}\right)}\right\}} \tag{3.13}
\end{equation*}
$$

In the above equation $\mu_{l}$ and $N_{l}$ are the chemical potential and the occupation number operator of the lead $l$.

The RDO is defined as the (partial) trace on the Fock space of the leads

$$
\begin{equation*}
\rho(t)=\operatorname{Tr}_{L} \operatorname{Tr}_{R} W(t), \quad \rho\left(t_{0}\right)=\rho_{S} \tag{3.14}
\end{equation*}
$$

To find the matrix elements of $\rho(t)$ with respect to a basis in the Fock space $\mathcal{F}_{S}$ of the sample we compute conditional reduced operators acting in different $n$-particle sectors of the Fock space. Li et al. (36) proposed a factorization for the full density matrix $\left(\rho(t)=\sum_{n} \rho^{(n)} \otimes \rho_{\text {leads }}\right)$ which generalizes the usual Born-Markov approximation. In our approach, we do not impose an equilibrium state on the leads after the coupling is switched on, which would mean to take $W(t)=\rho_{L} \rho_{R} \rho(t)$. We will use an occupation number basis constructed from the single electron states (SESs) of the isolated finite quantum wire $\left\{\psi_{a}^{S}\right\}$. The many electron state (MES) $\mu$ reads as follow

$$
\begin{equation*}
|\mu\rangle=\left|i_{1}^{\mu}, i_{2}^{\mu}, \ldots, i_{n}^{\mu}, \ldots\right\rangle \tag{3.15}
\end{equation*}
$$

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where the number $i_{n}^{\mu}$ indicates if the $n$-th single particle state is occupied $\left(i_{n}^{\mu}=1\right)$ or empty $\left(i_{n}^{\mu}=0\right)$. The corresponding energy of the noninteracting many-body state is represented by $\mathcal{E}_{\mu}$ and is given by the sum of the occupied single-particle levels, $\mathcal{E}_{\mu}=\sum_{a} E_{a} i_{a}^{\mu}$. If the central region contains $N \sim 20$ electrons the size of the reduced density matrix becomes very large and for $N \sim 50$ it seems quite impossible to compute the entire matrix, even within the Markov approximation. We consider that the number of MESs that are relevant to the transport problem can actually be much smaller, and at low temperatures it is controlled by the bias applied to the leads. In the present model the bias is included as the difference between the chemical potentials of the leads i.e. $\mathrm{eV}=\mu_{L}-\mu_{R}$, a procedure which is also used in the Keldysh formulation of electronic transport $(37 ; 38)$. We assume now that at an initial instant $t_{0}$ the density operator of the central region is such that the first $N_{0}$ single-particle states are occupied and all the higher states are empty, that is

$$
\begin{equation*}
\rho\left(t_{0}\right)=\left|\mu_{0}\right\rangle\left\langle\mu_{0}\right|, \quad\left|\mu_{0}\right\rangle=|\underbrace{1,1, \ldots .1}_{N_{0} \text { states }}, 0,0, \ldots .\rangle \tag{3.16}
\end{equation*}
$$

where $\mu_{0}$ is just the label of the selected many-body state. When the leads are connected to the central region the following situation is expected: 1) The lowest $N_{0}$ levels remain occupied and will not contribute to transport. 2) We assume that electrons tunnel through the dot only via the levels located in the energy range $\left[\mu_{R}-\delta, \mu_{L}+\delta\right]$. 3) In the transient regime the occupation numbers of these states will depend on time and will eventually settle down in a steady-state regime. Taking into account all of these it is clear that there are only $\left(N_{\max }-N_{0}\right)$ singleparticle states which are active in the transport process and consequently it is sufficient to compute only the matrix elements of the RDO for the $\mathcal{N}=2^{N_{\max }-N_{0}}$ many-body states having the following form

$$
\begin{equation*}
|\mu\rangle=|\underbrace{1,1, \ldots .1}_{N_{0} \text { states }}, i_{N_{0}+1}^{\mu}, \ldots, i_{N_{\max }}^{\mu}, 0,0, \ldots .\rangle \tag{3.17}
\end{equation*}
$$



Figure 3.1: The initial configuration in the many-level quantum dot for a given pair of chemical potentials on the leads $\mu_{L}, \mu_{R}$ and a 'gap' $\delta$. The occupied levels are marked by thick lines.

This assumption of us about relatively few active transport states has to be numerically investigated for each particular model of interest.

### 3.2 Time evolution

### 3.2.1 Derivation of GME

By using using the superoperator method developed by Haake (39) and the notation $U(t)=e^{\left(H_{S}+H_{\text {leads }}\right) / i \hbar}$ for the unitary propagator associated to the disconnected system we obtain the following GME for the reduced density operator up to second order in the tunneling Hamiltonian in the kernel of the integro-differential equation

$$
\begin{align*}
\dot{\rho}(t)= & -\frac{i}{\hbar}\left[H_{\mathrm{S}}, \rho(t)\right] \\
& -\frac{1}{\hbar^{2}} \sum_{l=\mathrm{L}, \mathrm{R}} \int d q \chi_{l}(t)\left(\left[\mathcal{T}_{l}, \Omega_{q l}(t)\right]+h . c .\right), \tag{3.18}
\end{align*}
$$

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where we have introduced two operators to compactify the notation

$$
\begin{aligned}
& \Omega_{q l}(t)=U_{\mathrm{S}}^{\dagger}(t) \int_{t_{0}}^{t} d s \chi_{l}(s) \Pi_{q l}(s) e^{i((s-t) / \hbar) \varepsilon_{l}(q)} U_{\mathrm{S}}(t) \\
& \Pi_{q l}(s)=U_{\mathrm{S}}(s)\left(\mathcal{T}_{l}^{\dagger} \rho(s)\left(1-f_{l}\right)-\rho(s) \mathcal{T}_{l}^{\dagger} f_{l}\right) U_{\mathrm{S}}^{\dagger}(s)
\end{aligned}
$$

and a scattering operator $\mathcal{T}$ acting in the many-electron Fock space of the system

$$
\begin{align*}
\mathcal{T}_{l}(q) & =\sum_{\alpha, \beta} \mathcal{T}_{\alpha \beta}^{l}(q)|\alpha\rangle\langle\beta| \\
\mathcal{T}_{\alpha \beta}^{l}(q) & =\sum_{a} T_{a q}^{l}\langle\alpha| d_{a}^{\dagger}|\beta\rangle \tag{3.19}
\end{align*}
$$

$\mathcal{T}_{\alpha \beta}^{l}(q)$ describes the 'absorption' of electrons from the leads to the system and changes the many-electron state of the latter from $\beta \rightarrow \alpha$. The Fermi function of the SES labelled by $q \leftrightarrow\left(n_{y}^{l} q\right)$ in lead $l$ is noted by $f_{l}(\epsilon(q))=\left\{\exp \left[\epsilon(q)-\mu_{l}\right] / k T+1\right\}^{-1}$.

More details about the derivation of GME are given in Appendix A.

### 3.2.2 Observables

With the RDO it is now possible to compute the statistical average of the charge operator in the coupled sample $Q_{S}=e \sum_{n} d_{n}^{\dagger} d_{n}$

$$
\begin{align*}
\left\langle Q_{S}(t)\right\rangle & =\operatorname{Tr}\left\{W(t) Q_{S}\right\}=\operatorname{Tr}_{S}\left\{\left[\operatorname{Tr}_{L R} W(t)\right] Q_{S}\right\} \\
& =\operatorname{Tr}_{S}\left\{\rho(t) Q_{S}\right\}=e \sum_{a, \mu} i_{a}^{\mu}\langle\mu| \rho(t)|\mu\rangle \tag{3.20}
\end{align*}
$$

with the traces assumed over the Fock space. We are also interested in the average spatial distribution of the time-dependent charge

$$
\begin{equation*}
\left\langle Q_{S}(\mathbf{r}, t)\right\rangle=e \sum_{a b} \sum_{\mu \nu} \Psi_{a}^{*}(\mathbf{r}) \Psi_{b}(\mathbf{r}) \rho_{\mu \nu}(t)\langle\nu| d_{a}^{\dagger} d_{b}|\mu\rangle \tag{3.21}
\end{equation*}
$$

Then we define the net currents in the leads as follows $J_{L}(t)=-\frac{d Q_{L}}{d t}$ and $J_{R}(t)=\frac{d Q_{R}}{d t}$. We therefore have $J_{L}>0$ if the electrons flow from the left lead towards the sample and $J_{R}>0$ if they flow from the sample towards the right lead. It is more convenient to consider positive the currents flowing from left to right at both contacts and negative if the flow from right to left. Therefore in the following we will define $J_{R}(t)=$ $-\frac{d Q_{R}}{d t}$. In the transient regime the sign of the net currents can change. The continuity equation reads

$$
\begin{align*}
J(t) & =J_{L}(t)-J_{R}(t)=\frac{d\left\langle Q_{S}(t)\right\rangle}{d t} \\
& =\sum_{n} \sum_{\nu} i_{n}^{\nu}\langle\mu| \dot{\rho}(t)|\mu\rangle \tag{3.22}
\end{align*}
$$

In the steady state, i.e. for $(t \rightarrow \infty)$ the charge in the sample $Q_{S}(t)$ is constant and thus $J(t)=0$. This means the current entering the sample equals the current exiting the sample, $J_{L}(t)=J_{R}(t)$.

Through the GME (3.18) it is possible to identify the contribution of each SES in the system to the current from the left lead or into the right lead.

## 4

## Time Dependent Transport

### 4.1 Transient and steady states

In order to describe the gradual coupling of the leads to the sample (with the length $L_{x}=900 \mathrm{~nm}$ ) we use specific coupling functions $\chi_{l}(t)$, with $l=L, R$. Initially, the coupling of both leads is defined by $\chi_{l}(t)=$ $1-2 /\left(e^{\gamma t}+1\right)$, where the parameter $\gamma=1.0 \mathrm{ps}^{-1}$ defines the smoothness of the coupling. The parameters determining the coupling of the subsystems in the function $g_{a q}^{l}$ (equation 3.8, and 3.11) are: $\delta_{1} a_{w}^{2}=1.0$, and $\delta_{2} a_{w}^{2}=2.0$. For the numerical coupling constant $g_{0}^{l}$, we select the value $g_{0} a_{w}^{3 / 2}=926.0 \mathrm{meV}$ for both leads. The unusual dimension of the numerical coupling constant comes from the fact that the $x$ part of the wave function in the leads is only $\delta$-normalizable. The effective coupling of the states in the leads and the central sample are much "smaller" since the contact areas are only a small fraction of the total area of the central system. In the next two subsections of this chapter we focus our attention on the effects of these parameters.

Later, when we will investigate turnstile pumping we shall introduce an alternative form for $\chi_{l}(t)$.

## 4. TIME DEPENDENT TRANSPORT

### 4.1.1 Pure finite quantum wire

To explore the properties of the system we study the time-dependent transport of electrons through it. The energy spectrum of the leads and of the sample are shown in Figure 4.1. The maximum energy for each subband shown in the graph indicates the corresponding maximum wave vector in the $q a_{w}$-integration of the GME. The chemical potentials in the leads defining the bias window (BW) are shown with the dotted horizontal lines. We consider $\mu_{L}=1.0 \mathrm{meV}$ and $\mu_{R}=0.85 \mathrm{meV}$ with the limits $\mu_{R}-\Delta$ and $\mu_{L}+\Delta$ with $\Delta=0.15 \mathrm{meV}$ defining the window of relevant states around the applied bias $e V_{\text {bias }}=\mu_{L}-\mu_{R}=0.15$ meV . The states with energies below $\mu_{R}-\Delta$ will be considered totally and permanently occupied and the states with energies above $\mu_{L}+\Delta$ will be considered totally empty. The states with energy in the interval [ $\mu_{R}-\Delta, \mu_{L}+\Delta$ ] will be considered active in transport.
In the present example the active window contains 4 SESs while the bias window includes 1 SES.


Figure 4.1: The energy spectrum of the leads vs. the scaled wave vector $q a_{w}$ (red). The subband index is $n=0,1$. The energy spectrum of the isolated sample ( $L_{x}=900 \mathrm{~nm}$ ) with crosses. With horizontal narrow dotted lines (green) the chemical potentials $\mu_{L}=1.0 \mathrm{meV}$ and $\mu_{R}=0.85$ meV and with horizontal wide dashed lines the limits $\mu_{R}-\Delta$ and $\mu_{L}+\Delta$ with $\Delta=0.15 \mathrm{meV}, B=0 \mathrm{~T}$.

In Figure 4.2 we display both currents in the leads: the current entering the system from the left lead, and the current exiting the system into the right lead, when the system is initially empty and also when it contains one electron. We see that in the case of the initially empty system, the current in the right lead, is negative meaning that it is directed into the system for $t<60 \mathrm{ps}$. When the system is initially occupied by one electron, in the lowest active state $a=6$, we see fluctuations in the right current for $t<20 \mathrm{ps}$ before it turns positive when a net current is flowing through the system (since there are two states below $\mu_{R}$ ).


Figure 4.2: The total current from the left lead, and the total current from the right lead for an initially empty system and a system with one electron initially in equilibrium. $L_{x}=900 \mathrm{~nm}, B=0 \mathrm{~T}$.

The time-dependent occupation of each sample state included in the calculation is shown in Figure 4.3; we also indicate the functions $\chi_{l}(t)$. The states are $6,7,8,9$ in the order of increasing energy shown with crosses in Figure 4.1. We note that some of the higher SESs seem to reach a steady state fast, while the ones lower in energy are still increasing their occupation at times as large as 120 ps. This happens because the higher lying states are stronger coupled to states in the leads and they can conduct faster. We see that in case of one electron initially in the system there is a finite but small probability for the electron to get out of the system, even though it has energy below the actual bias window.

## 4. TIME DEPENDENT TRANSPORT



Figure 4.3: The time dependent occupation of the relevant SESs for an initially empty system (a), and for a system occupied with initially one electron (b). The time coupling functions $\chi_{l}(t)$, with $l=L, R$, are shown for reference (wide dashed black curves). $L_{x}=900 \mathrm{~nm}, B=0 \mathrm{~T}$.


Figure 4.4: The average spatial charge distribution for the MES constructed from the four relevant SESs in the quantum wire, at different time moments. The system is initially empty. $L_{x}=900 \mathrm{~nm}, B=0 \mathrm{~T}$.

As expected, the system looses the electron occupying the SES, $a=7$, (this state is situated below $\mu_{R}$ ).

Using the reduced density operator we calculate the average spatial charge distribution of the MES in the finite quantum wire at any instant of time. In Figure 4.4 we show it for different times. Soon after the coupling of the system to the leads ( $t=5.3 \mathrm{ps}$ ), the probability density increases from both sides of the wire. When the system reaches a steady state ( $t=182.3 \mathrm{ps}$ ), we see that the coupling to the leads maintains a higher probability at the ends of the finite wire.

### 4.1.2 Quantum Point Contacts

## One Quantum Point Contact (QPC)

Now, because we want to explore the effects of the geometry of the system on the transport, we introduce a QPC into the finite quantum wire. Geometrically a quantum point contact is a constriction that can be simulated by two Gaussian potentials as long as we are describing electrons in a finite energy range

$$
\begin{equation*}
W(x, y)=V_{1} e^{\left[-\beta_{x, 1}\left(x-x_{1}\right)\right]^{2}-\left[\beta_{y, 1}\left(y-y_{1}\right)\right]^{2}}+V_{2} e^{\left[-\beta_{x, 2}\left(x-x_{2}\right)\right]^{2}-\left[\beta_{y, 2}\left(y-y_{2}\right)\right]^{2}} \tag{4.1}
\end{equation*}
$$

with the parameters $V_{1}=V_{2}= \pm 6.5 \mathrm{meV}$ and $\beta_{x}=\beta_{y}=0.03 \mathrm{~nm}^{-1}$. The contour of the potential defining this system can be seen in Figure 4.5.

In Figure 4.6, the energy spectrum of the SES is shown for a QPC for the potential given by equation (4.1) and compared to the case for a pure wire. We select the chemical potentials in each lead and the extended bias window in a such way to include the same SESs like in the case for a pure wire.

## 4. TIME DEPENDENT TRANSPORT



Figure 4.5: The potential for a quantum wire with a single Quantum Point Contact. $L_{x}=900 \mathrm{~nm}, B=0 \mathrm{~T}$.


Figure 4.6: The energy spectrum of the isolated sample with a QPC ( $L_{x}$ $=900 \mathrm{~nm})$. With horizontal narrow dashed lines the chemical potentials $\mu_{L}=1.06 \mathrm{meV}$ and $\mu_{R}=0.86 \mathrm{meV}$ and with horizontal wide dashed lines the limits $\mu_{R}-\Delta$ and $\mu_{L}+\Delta$ with $\Delta=0.1 \mathrm{meV}$.

We show also the currents from the left and right lead, corresponding to these states in Figures 4.8 and 4.9.


Figure 4.7: The total current from the left lead, and the total current from the right lead for an initially empty system. The system contains One QPC respectively no QPC. $L_{x}=900 \mathrm{~nm}$.


Figure 4.8: The partial current from the left lead (a) respectively from the right lead (b) for an initially empty system. The system contains no QPC. $L_{x}=900 \mathrm{~nm}$.

When we have a QPC (Figure 4.9), the current into the state with the lowest energy, $a=6$, reaches a steady state after a long time relatively to other states because the coupling between the wire and the leads is stronger for these higher states as shown in Figure 4.12.

We look at the charge distribution, for the system which contains a

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Figure 4.9: The partial current from the left lead (a) respectively from the right lead (b) for an initially empty system. The system contains one QPC. $L_{x}=900 \mathrm{~nm}$.
$\operatorname{QPC}\left(V_{1}=V_{2}=6.5 \mathrm{meV}\right)$, before and after the system has reached a steady state (Figure 4.10). Soon after the initial coupling ( $t=5.3 \mathrm{ps}$ ), we see electron probability seeping in from both contact regions, though more from the higher bias region at the left. In the steady state regime ( $t=197.5 \mathrm{ps}$ ), the electrons have a higher probability to be found around the constriction.


Figure 4.10: The average spatial charge distribution for the system embedded with a QPC, at different time moments. The system is initially empty. $L_{x}=900 \mathrm{~nm}$.

In Figure 4.11, for a double dot cavity $\left(V_{1}=V_{2}=-6.5 \mathrm{meV}\right)$, at
$t=5.3 \mathrm{ps}$, we see the charge seeping into the system from both contact regions, like before, but now no extra probability is seen close to the constriction. The steady state attained in the end $(t=197.5 \mathrm{ps})$ is a mixed state with contribution from all of the available SESs, and the coupling to the leads maintains a higher probability at the ends of the finite wire.


Figure 4.11: The average spatial charge distribution for the system embedded with a double dot cavity, at different time moments. The system is initially empty. $L_{x}=900 \mathrm{~nm}$.

It is interesting to view in Figure 4.12 the probability density of the relevant SESs. There we see that the SES $a=7$ and $a=9$ have a high probability in the constriction but a much reduced probability density toward the contact ends of the system. The emergence of a higher charge density in the constriction of the QPC in Figure 4.10 could thus be viewed like a formation of a broad resonance state. A phenomenon that has been observed in models built on scattering approaches to transport, like Lippmann-Schwinger formalism.

To mark out the effects of the next subband we select the location of the bias window just below and touching the second subband of the system (Figure 4.13). The position of arrows indicates for which number of state we plot in Figure 4.14 the probability density.


Figure 4.12: The probability density of the single-electron eigenstates of the system embedded with a QPC. $L_{x}=900 \mathrm{~nm}$.


Figure 4.13: The energy spectrum of the isolated sample with a QPC ( $L_{x}$ $=900 \mathrm{~nm})$. With horizontal narrow dashed lines the chemical potentials $\mu_{L}=1.45 \mathrm{meV}$ and $\mu_{R}=1.3 \mathrm{meV}$ and with horizontal wide dashed lines representing the limits $\mu_{R}-\Delta$ and $\mu_{L}+\Delta$ with $\Delta=0.15 \mathrm{meV}$.


Figure 4.14: The probability density of the single-electron eigenstates of the system embedded with a QPC. $L_{x}=900 \mathrm{~nm}$.

For $a=12$ and $a=13$ the electron probability has a character of a state of the second subband, but it is very interesting what happens for $a=14$; it has a character of a state from the first subband.

Generally, the steps seen in the current in Figure 4.7 are indicative of the presence of more than one active transport state. The different dynamical behavior of the states and the competition between them leads to the steps.

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## Double Quantum Point Contact

A double QPC is made up of two QPCs which are positioned in series. A cavity is formed between the QPCs that can capture electrons in quasibound states. We represent a double QPC with the following form

$$
\begin{align*}
W(x, y) & =V_{1} e^{\left[-\beta_{x, 1}\left(x-x_{1}\right)\right]^{2}-\left[\beta_{y, 1}\left(y-y_{1}\right)\right]^{2}}+V_{2} e^{\left[-\beta_{x, 2}\left(x-x_{2}\right)\right]^{2}-\left[\beta_{y, 2}\left(y-y_{2}\right)\right]^{2}} \\
& +V_{3} e^{\left[-\beta_{x, 3}\left(x-x_{3}\right)\right]^{2}-\left[\beta_{y, 3}\left(y-y_{3}\right)\right]^{2}}+V_{4} e^{\left[-\beta_{x, 4}\left(x-x_{4}\right)\right]^{2}-\left[\beta_{y, 4}\left(y-y_{4}\right)\right]^{2}} \tag{4.2}
\end{align*}
$$

with the parameters $V_{1}=V_{2}=V_{3}=V_{4}=6.5 \mathrm{meV}$ and $\beta_{x}=\beta_{y}=0.03$ $\mathrm{nm}^{-1}$.

The system with embedded double QPC can be seen in Figure 4.15.


Figure 4.15: The potential for a quantum wire with two Quantum Point Contacts. $L_{x}=900 \mathrm{~nm}$.

The energy spectrum for this system is shown in Figure 4.16 in comparison with a system containing one QPC. Here we keep the same SESs as before, and in addition the energy spectrum gives us the possibility to select the same chemical potentials in leads as in the case for one QPC.

We use this opportunity to show the difference between the total currents from both leads when the system includes one and two QPCs


Figure 4.16: The energy spectrum of the isolated sample with a double QPC ( $L_{x}=900 \mathrm{~nm}$ ). With horizontal narrow dashed lines the chemical potentials $\mu_{L}=1.06 \mathrm{meV}$ and $\mu_{R}=0.86 \mathrm{meV}$ and with horizontal wide dashed lines the limits $\mu_{R}-\Delta$ and $\mu_{L}+\Delta$ with $\Delta=0.1 \mathrm{meV}, B=0 \mathrm{~T}$.
(Figure 4.17). The double QPC may considerably slow down the transient processes and affects the shape of the currents; the amplitude of the currents is smaller. The same statement could be true for the partial


Figure 4.17: The total current from the left lead, and the total current from the right lead for an initially empty system. The system contains one respectively two QPCs. $L_{x}=900 \mathrm{~nm}, B=0$.
currents, where in Figure 4.18 we analyze the current corresponding to the 8th state (this state is situated in the bias window, see Figure 4.16).

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Figure 4.18: The partial currents into the state $a=8$ from the left lead (a) respectively from the right lead (b) for an initially empty system. The system contains one respectively two QPCs. $L_{x}=900 \mathrm{~nm}$.

The explanation is given by the coupling strength tensor, which gives the coupling between a state $a$ in the relevant extended bias window and a state $q n_{y}$ in the leads (the coupling is the same for left and right lead). In Figure 4.19, we see that when we have two QPCs the coupling which corresponds to the 8th state is weaker in contrast to the case of one QPC in the wire.


Figure 4.19: The coupling tensor between the states situated in the sample and states of the lowest subband in the leads for one (left), and respectively two QPCs (right). $L_{x}=900 \mathrm{~nm}$.

We have seen the properties of the system affected by the band struc-
ture in the neighborhood of the first and of the bottom of the second subband. The question is what happens with the bottom of the first subband? There the states in the sample are less coupled to the states in the leads and carry a smaller amount of a current.

In Figure 4.20 we show again the energy spectrum of a system embedded with a double QPC together with the chemical potentials selected but here just the bound state of the well is below the bias window. We show the time-dependent occupation of the SESs, and we see that the system is far from reaching a steady state for $\operatorname{SES} a=2$ and $a=3$; the occupation of the levels is still growing linearly (Figure 4.21(a)). This can also be verified by observing the partial left current for the relevant SESs in Figure 4.21(b).

Even though the density of states is high close to the band edge, the group velocity of the states is very low, and in addition the low energy eigenstates in the central system and the leads do not penetrate strongly into the contact region leading to low current.


Figure 4.20: The energy spectrum of the isolated sample with a double QPC. With horizontal narrow dashed lines the chemical potentials $\mu_{L}=$ 0.6 meV and $\mu_{R}=0.52 \mathrm{meV}$ and with horizontal wide dashed lines the limits $\mu_{R}-\Delta$ and $\mu_{L}+\Delta$ with $\Delta=0.07 \mathrm{meV} . L_{x}=900 \mathrm{~nm}$.

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Figure 4.21: The time dependent occupation of the relevant SESs (a) and the partial current from the left lead (b) for an initially empty system. The system contains two QPCs. $L_{x}=900 \mathrm{~nm}$.

### 4.2 Modulated currents

In this section we see how the time-dependent coupling of the left lead to the system is used to generate a signal which is observed in the right lead. That the GME formalism can be used to describe this is not all obvious but will be verified here.

In order to describe the gradual coupling of the leads to the sample (with the length $L_{x}=300 \mathrm{~nm}$ ) and the periodic modulation of the left contact we use specific coupling functions $\chi_{l}(t)$, with $l=L, R$ (see Figure 4.22). The coupling to the leads begins at $t=0$ and evolves in time. After some time $t_{0}>0$ the coupling to the left lead is turned off and on periodically while the right lead is always connected to the system.

### 4.2.1 Delay of the output signal

In this subsection we show the results in the absence of the magnetic field.

The energy spectrum of the leads and of the sample are shown in Figure 4.23. The maximum energy for each subband shown in the graph indicates the corresponding maximum wave vector in the $q a_{w}$-integration


Figure 4.22: The time coupling functions $\chi_{l}(t)$, with $l=\mathrm{L}$ (red), R (blue). $T=60 \mathrm{ps}$.
of the GME. The chemical potential in the leads defining the bias window (BW) are shown with the dashed horizontal lines. We consider two BW's: BW1 with chemical potentials $\mu_{L}=1.48 \mathrm{meV}$ and $\mu_{R}=0.78 \mathrm{meV}$, and BW2 with $\mu_{L}=2.48 \mathrm{meV}$ and $\mu_{R}=1.78 \mathrm{meV}$ respectively. In both cases the applied bias is $e V_{\text {bias }}=\mu_{L}-\mu_{R}=0.70 \mathrm{meV}$. We also include the sample states with energy outside the BW, between the limits $\mu_{R}-\Delta$ and $\mu_{L}+\Delta$ with $\Delta=0.1 \mathrm{meV}$.
The first active window contains 4 SESs and the second one contains 5 SESs.

In Figure 4.24 we show the time-dependent total occupation of the relevant SESs for BW1 and BW2. We also indicate the functions $\chi_{l}(t)$. In this example the parameters characterizing the coupling of the sample to the leads are: $g_{0} a_{w}^{3 / 2}=926.0 \mathrm{meV}, \delta_{1} a_{w}^{2}=1.0$, and $\delta_{2} a_{w}^{2}=2.0$.
For the higher bias window (BW2) we see that more charge is transferred through the system in comparison with the lower one. The reason for that is that BW2 includes three subbands of the leads, while BW1 includes only two (see Figure 4.23). In addition, the higher lying states penetrate stronger into the contact region leading to stronger coupling.

In Figure 4.25 we plot again the energy spectrum but now for a higher chemical potential of the left lead. The reason for doing this is


Figure 4.23: The energy spectrum of the leads vs. the scaled wave vector $q a_{w}(B=0 \mathrm{~T})$. The subband index is $n=0,1,2,3$. With crosses the energy spectrum of the isolated sample ( $L_{x}=300 \mathrm{~nm}$ ). With horizontal wide dashed lines the chemical potentials $\mu_{L}=1.48 \mathrm{meV}$ and $\mu_{R}=0.78$ (BW1), and with horizontal narrow dashed lines $\mu_{L}=2.48 \mathrm{meV}$ and $\mu_{R}=1.78 \mathrm{meV}$ (BW2).


Figure 4.24: The time dependent total occupation of the relevant SESs for a system occupied initially with 1 electron for the first (solid), and second (dotted) bias window. The time coupling functions $\chi_{l}(t)$, with $l=L, R$, are shown for reference. Other parameters: $g_{0} a_{w}^{3 / 2}=926 \mathrm{meV}$, $\delta_{1} a_{w}^{2}=1.0, \delta_{2} a_{w}^{2}=2.0$, and $T=60 \mathrm{ps} . L_{x}=300 \mathrm{~nm}$.
that we want to include in the BW2 three SESs (we shall discuss later this reason).


Figure 4.25: The energy spectrum of the isolated sample ( $L_{x}=300 \mathrm{~nm}$ ). The chemical potentials are $\mu_{L}=2.54 \mathrm{meV}$ and $\mu_{R}=1.78$.

The currents depend strongly on the pulse length. To underline that we show in Figure 4.26 the time-dependent total currents in both leads for different pulse length ( $\mu_{L}=2.54 \mathrm{meV}$ and $\mu_{R}=1.78 \mathrm{meV}$ ). In the beginning the system is coupled to the leads and both contacts are kept open for a time $t_{0}$. Then the the left contact is modulated by pulses while the other one is left open. The four signals do not drop at the same time because of the different shifts $\tau$ used in the construction of $\chi_{L}(t)$ (we have $\tau_{L}=30 \mathrm{ps}, 45 \mathrm{ps}, 55 \mathrm{ps}$ and 75 ps ). The first observation is that for very short pulses ( $T=10 \mathrm{ps}$ in Figure $4.26(\mathrm{a})$ ) the input current $J_{L}$ has a triangular shape although the modulating signal is rectangular. In addition $J_{R}$ does not vanish when the left lead is disconnected.
When the pulse length increases the shape and the amplitude of the output current change considerably. $J_{R}$ reaches maxima even before the pulse is turned off and remains almost constant during the second half of the pulse. We notice that right after the left contact opens the current from the left lead is injected in the sample quite fast but the current in the right lead increases slower.
In Figure $4.26(\mathrm{~d})$ we see that if we increase further the pulse length,

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the amplitude of the output current increases too, but still does not reproduce the input signal.


Figure 4.26: The total current entering the system from the left lead and the total current exiting the system into the right lead for four pulses (a) $T=10 \mathrm{ps}, \mathrm{b}) 40 \mathrm{ps}$, c) 60 ps and d) 100 ps . Parameters: $g_{0} a_{w}^{3 / 2}=926.0$ $\mathrm{meV}, \delta_{1} a_{w}^{2}=1, \delta_{2} a_{w}^{2}=2$ and $\mu_{L}=2.54 \mathrm{meV}$ and $\mu_{R}=1.78 . L_{x}=300$ nm .

In Figure 4.27 we compare the total charge accumulated on the 5 SESs within the bias window for the four pulse lengths. As the pulse length increases more charge is transferred through the system and therefore the output current increases. We notice that for the 60 ps and 100 ps pulses, the charge relaxes exponentially (by increasing the pulse length, the left lead feeds enough charge to the sample).

We present in Figure 4.28 the snapshots of charge density for the configuration which is presented in Figure 4.26(c). The charge distribution


Figure 4.27: The total charge accumulated on the 5 SESs from the bias window for the four pulse lengths considered in Figure 4.26. $L_{x}=300 \mathrm{~nm}$.
reflects the geometry of the 5 SESs within the bias window and provides interesting information on the electronic propagation in the system. We show it soon after the coupling of the system to the leads at $t=1.52$ ps (here the distribution of the charge is the same in both ends of the sample). If we compare the scale, at $t=14.43 \mathrm{ps}$ more charge is accumulated in the system and the distribution is more pronounced in the right part of the central region; to explain that we analyze the currents and we see that at this time the current from the left decreases while the right one increases. For the next three snapshots we have a similar situation, but if we take a look on the scales the charge does not change because between these intervals the occupation number reaches steady state (see Figure 4.27 - blue line). At $t=68.36 \mathrm{ps}$ is very easy to see that the probability is smaller because the occupation number started to decrease; when the occupation increases again we would expect to see a higher probability (at $t=101.79 \mathrm{ps}$ ).








Figure 4.28: The average spatial charge distribution in the quantum wire for $B=0 \mathrm{~T}$, at different time moments. $T=60 \mathrm{ps} . L_{x}=300 \mathrm{~nm}$.

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### 4.2.2 Effects of magnetic fields

In the presence of a magnetic field we expect the amplitude of the charge oscillations to decrease. The reason is that the electronic trajectories can bend due to the Lorentz force and the electrons might return to the source lead rather than traveling directly to the drain lead. At the same time we should though remember that generally backscattering is reduced by magnetic field, as has been seen in studies using the Lippmann Schwinger formalism.

We show the results for the same parameters as before, which characterized the coupling of the sample to the leads $\left(g_{0} a_{w}^{3 / 2}=926.0 \mathrm{meV}\right.$, $\delta_{1} a_{w}^{2}=1.0$, and $\delta_{2} a_{w}^{2}=2.0$ ) and we keep also the same number of SESs (like before - Figure 4.25). We select the bias windows with three states included in the windows and two marginal states in the extended regions but now the bias window is different in comparison with $B=0 \mathrm{~T}$ because for each new magnetic field we get a new energy spectrum.

In Figure 4.29(a) we see that the transfer of the electrons decreases with increasing the magnetic field. For $B=0 \mathrm{~T}$ an amount of charge $Q_{p} \approx 0.9$ electron can be transmitted along the wire sample in one cycle, and for $B=0.2 \mathrm{~T} Q_{p} \approx 0.6$. For stronger magnetic fields $Q_{p}$ drops to 0.4 for $B=0.4 \mathrm{~T}$, and $Q_{p}<0.25$ at $B>0.6 \mathrm{~T}$.

To have a better idea about what happens, in Figure 4.29(b), and (c) we plot the currents in the left respectively right lead. Both currents decrease with increasing the magnetic field. We saw that the presence of the magnetic field reduces the electron transfer, but the charge still increases with increasing coupling between the leads and the sample (see Figure 4.30). The parameters for the coupling are: $g_{0} a_{w}^{3 / 2}=1200 \mathrm{meV}$, $\delta_{1} a_{2}^{2}=0.75$, and $\delta_{2} a_{w}^{2}=1.5$. These parameters correspond to the same physical parameters that were used for $B=0 \mathrm{~T}$, as $a_{w}$ depends on $B$.

In Figure 4.31 we analyze both currents in the leads for $B=1 \mathrm{~T}$. For this value and for each value of the magnetic field we obtain the same effect: the shape of the pulse can be reproduced by the output signal.




Figure 4.29: (a) The time dependent total occupation of the relevant SESs for different values of the magnetic field. The total current from the left lead (b) and the total current into the right lead (c). $g_{0} a_{w}^{3 / 2}=926$ $\mathrm{meV}, \delta_{1} a_{w}^{2}=1.0, \delta_{2} a_{w}^{2}=2.0, T=60 \mathrm{ps} . L_{x}=300 \mathrm{~nm}$.


Figure 4.30: The time dependent total occupation of the relevant SESs for $B=0.9-1.2 \mathrm{~T} . g_{0} a_{w}^{3 / 2}=1200 \mathrm{meV}, \delta_{1} a_{2}^{2}=0.75$, and $\delta_{2} a_{w}^{2}=1.5$, $T=60 . L_{x}=300 \mathrm{~nm}$.

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Figure 4.31: The total current entering the system from the left lead and the total current exiting the system into the right lead. $g_{0} a_{w}^{3 / 2}=1200$ $\mathrm{meV}, \delta_{1} a_{2}^{2}=0.75$, and $\delta_{2} a_{w}^{2}=1.5, T=60 \mathrm{ps} . L_{x}=300 \mathrm{~nm}$.


Figure 4.32: The partial current from the left lead (a) respectively from the right lead (b) for $B=1.0 \mathrm{~T}$. Other parameters: $g_{0} a_{w}^{3 / 2}=1200 \mathrm{meV}$, $\delta_{1} a_{2}^{2}=0.75$, and $\delta_{2} a_{w}^{2}=1.5 . T=60 \mathrm{ps} . L_{x}=300 \mathrm{~nm}$.

In the following we compare the partial currents in the left (right) lead for $B=1.0 \mathrm{~T}$ in the case of the long pulse, $(T=60 \mathrm{ps})$. The currents entering the sample from the left lead (see Figure 4.32(a)) have interesting features: the currents corresponding to the 7th, 8th and 9th state rise suddenly to a maximum value, while the currents to the 6th and 10th state increase slower and do not reach a maximum within the pulse duration. This suggests that the lowest and highest state absorb less charge from the left reservoir.
The partial currents $J_{R}(t)$ (Figure $4.32(\mathrm{~b})$ ) confirm that the 6 th and 10th state do not contribute significantly to the transport.

By looking at the occupation numbers shown in Figure 4.33 one convinces himself that this is indeed the case. The states 6 and 10 are slightly outside the BW and obviously their contribution to the transport is smaller.


Figure 4.33: The time dependent total occupation of the relevant SESs for $B=1.0$ T. $g_{0} a_{w}^{3 / 2}=1200 \mathrm{meV}, \delta_{1} a_{w}^{2}=0.75$, and $\delta_{2} a_{w}^{2}=1.5 . T=60$ ps. $L_{x}=300 \mathrm{~nm}$.

### 4.3 Turnstile pumping

An important feature of the turnstile configuration is that the pumped current has a definite direction due to the finite bias. It is important to

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remind the reader that the concept of parametric charge pumping was introduced in the context of a net current in an unbiased system. We review the effects of the bias window, pulse length, and magnetic field on the evolution in time of the number of electrons in the sample. We select the parameters describing the coupling of the leads to the wire in two different ways, both scaled and not scaled with the effective width of the sample, which depends on the magnetic field. As in our previous sections describing the gradual coupling of the leads to the sample (with the length $L_{x}=300 \mathrm{~nm}$ ) we define analytically the coupling functions $\chi_{l}(t)$, with $l=L, R$. First time we switch off the left contact the right one is still kept on, then the the left is turned on again while the right is turned off (40) (see Figure 4.34).


Figure 4.34: The time coupling functions $\chi_{l}(t)$, with $l=\mathrm{L}$ (red), $\mathrm{R}(\mathrm{blue})$. $T=60 \mathrm{ps}$.

### 4.3.1 Effects of the bias

In this part we show the results in the absence of the magnetic field (using the same coupling of the sample to the leads as in the subsection 4.2.1: $\left.g_{0} a_{w}^{3 / 2}=926 \mathrm{meV}, \delta_{1} a_{w}^{2}=1.0, \delta_{2} a_{w}^{2}=2.0\right)$ and we underline the effects of the bias windows. In our calculations we keep the same number of states using the same chemical potentials in the leads which define the bias windows like in Fig. $4.23\left(\mu_{L}=1.48 \mathrm{meV}\right.$ and $\mu_{R}=0.78$ for BW1,

### 4.3 Turnstile pumping

respectively $\mu_{L}=2.48 \mathrm{meV}$ and $\mu_{R}=1.78 \mathrm{meV}$ for BW2 with $\Delta=0.1$ $\mathrm{meV})$.

In Figure 4.35 we show the time-dependent total occupation $n_{a}(t)$ of the relevant SES for BW1 and BW2. We also indicate the functions $\chi_{l}(t)$. The effects are similar like in the case for the modulated currents (see Figure 4.24) but now, in comparison with that, the number of the electrons for both bias windows increases because the contact from the right lead is not always connected to the system.


Figure 4.35: The time dependent total occupation of the relevant SES for a system occupied initially with 1 electron for the first and second bias window. The time coupling functions $\chi_{l}(t)$, with $l=L, R$, are shown for reference. Other parameters: $g_{0} a_{w}^{3 / 2}=926 \mathrm{meV}, \delta_{1} a_{w}^{2}=1.0, \delta_{2} a_{w}^{2}=2.0$, and $T=60 \mathrm{ps} . L_{x}=300 \mathrm{~nm}$.

It is interesting to observe the behavior of the states situated at the boundaries of the BW. To show that we choose the BW1 and display in Figure 4.37 respectively Figure 4.38 the partial currents and the occupations created by each state of the sample included in the calculations before and after changing the bias window. When the bias window is slightly pushed upwards ( $\mu_{L}=1.54 \mathrm{meV}$ instead of $\mu_{L}=1.48$ used in Figure 4.37(a) and Figure 4.38(a) the 4th enters the bias window (Figure 4.36). State 1 (the lowest cross) is considered totally occupied and frozen (it is not situated in the active region), states 3 and 4 are within

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the bias window while states 2 and 5 are situated in the extended window $\mu_{R}-\Delta$ and $\mu_{L}+\Delta$. When the state number 4 is included in the BW consequently the corresponding current increases. The current of state 5 also increases a bit, while the current associated to the other states does not change.


Figure 4.36: The energy spectrum of the isolated sample ( $L_{x}=300 \mathrm{~nm}$ ). The chemical potentials are $\mu_{L}=2.54 \mathrm{meV}$ and $\mu_{R}=1.78$.


Figure 4.37: The partial current entering the system from the left lead when the bias window contains one respectively two SESs. $T=60 \mathrm{ps}$. $L_{x}$ $=300 \mathrm{~nm}$.

By looking at the occupation number in Figure 4.38 we understand that the inclusion of one more state into the BW increases the occupation of the corresponding state and therefore the pumping. A similar behavior
is displayed by state number 9 situated on top of BW2 (not shown).


Figure 4.38: The time-dependent occupation for relevant SES when the bias window contains one respectively two SESs. $T=60 \mathrm{ps} . L_{x}=300$ nm .

Now we investigate the efficiency of the turnstile operation as a function of width of the bias window. We consider the case when the applied bias is $e V_{\text {bias }}=\mu_{L}-\mu_{R}=0.7 \mathrm{meV}$ (the first bias window), then we change the chemical potentials in the leads to get a new bias which is smaller or higher than BW1 ( $e V_{\text {bias }}=0.1,0.5$, and 0.9 meV$)$. So, if we now compare the results (see Figure 4.39(a)), the systematic observation is the following: as the bias window decreases or increases the total occupation of the parabolic wire decreases or increases as well respectively. The same statement is true for the total currents (Figure 4.39(b)).

To confirm what we said before we shall show the average pumped charge as a function of bias in Figure 4.40.

The efficiency of the turnstile operation depends on the pulse length $T$. The previous results are obtained with $T=60 \mathrm{ps}$. In those setups the system transfers at least two electrons per cycle. The present GME method is valid in the lowest (quadratic) order of the lead-sample coupling in the kernel of the integral equation, which means the tunneling of the electrons from the leads to the sample and back is a relatively


Figure 4.39: The time-dependent occupations and the currents from the right lead for different values of bias window. $T=60 \mathrm{ps} . L_{x}=300 \mathrm{~nm}$.


Figure 4.40: Pumped charge per cycle, vs. bias. $T=60 \mathrm{ps} . L_{x}=300$ nm .
slow process. Therefore by increasing or decreasing the pulse duration the transferred charge increases or decreases respectively. Denoting by $T_{t}$ the characteristic tunneling time, if $T \leq T_{t}$ the turnstile operation is not expected to work, the allowed time for the charging and discharging of the system being too short. This is the case for $T=10 \mathrm{ps}$ as shown in Figure 4.41, when clearly very little charge can enter and leave the system in a pumping cycle. Actually, the time $T_{t}$ depends on the pairwise coupling (or overlap) of each state of the leads to each state of the sample with energies within the BW. But in order to obtain significant pumping effects, the pulse duration has to include the time of flight (or propagation time) of electrons along the wire. This extra time depends on the energy of the electrons injected from the left lead.


Figure 4.41: The time dependent total occupation of the sample for three pulses at zero magnetic field. The trace for $T=60 \mathrm{ps}$ is the same as in Figure 4.35. $L_{x}=300 \mathrm{~nm}$.

Therefore, for a longer pulse, $T=40 \mathrm{ps}$, the turnstile pumping process is able to transfer charge through the sample. The occupation number has a triangular shape in time and it becomes periodic after 2-3 cycles. During the initial cycle, which includes the initial charging phase, the system accumulates more than 2 electrons and the steady state is already reached at about 30 ps when the charge in the system is saturated. This is possible because the right contact is still off. The right

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contact opens for the first time at 45 ps allowing more than 1 electron charge to pass into the right lead. For a longer period, like $T=60 \mathrm{ps}$, the occupation number develops toward a saw-tooth profile typical for the charging/relaxation processes. The asymmetry of the charge peaks is determined by the direction of the bias: the electrons leave the sample faster than they entered. The system drives almost two electrons from one lead into the other, which is remarkable given the length of our sample (300 nm).

### 4.3.2 Magnetic field and edge states

In order to compare our results at $B=0 \mathrm{~T}$ we first keep the same coupling parameters: $g_{0} a_{w}^{3 / 2}=926.0 \mathrm{meV}, \delta_{1} a_{w}^{2}=1.0$, and $\delta_{2} a_{w}^{2}=2.0$.

In Figure 4.42 we present the evolution of the total charge in the turnstile cycles at different values of the magnetic field and for each bias window. A technical detail has to be mentioned: for each value of the magnetic field the active window was adjusted such that the same states of the wire are contained in it. Moreover, the magnetic field is included in the leads as well so the subband structure changes.
As a general statement one can say that increasing the magnetic field the efficiency of the turnstile pump decreases. For $B=0 \mathrm{~T}$ and $B=0.2$ T more than one electron is still transmitted across the wire in one cycle, but then the pumped charge $Q_{p}$ drops to 0.7 for $B=0.4 \mathrm{~T}$, and finally $Q_{p}<0.3$ at $B=0.6 \mathrm{~T}$ and $B=0.8 \mathrm{~T}$ (for the first bias window). An interesting detail is that for BW2 is little difference between $B=0.6$ T and $B=0.8 \mathrm{~T}$ in comparison with BW1. It is also clear that for these coupling parameters, the charging time increases in the presence of the magnetic field. More precisely, there is less charge accumulated in the system in the normal switching regime ( $\chi_{L}=\chi_{R}, \mathrm{t}<60 \mathrm{ps}$ ) and, on the other hand, the charging process continues even after the pumping cycles starts. We should make two observations: one that it is clear that for BW2 the pumping is much better than for the BW1; for $B=0.2$

T we transfer $Q_{p}=1.3$ while for the first bias window we just have $Q_{p}=1$, because the coupling is much stronger for the states situated in the second BW (see Figure 4.43, where we should follow the scale on $z$ axis).


Figure 4.42: The time-dependent occupation of the relevant SESs for different magnetic fields: a) first bias window and b) second bias window. $T=60 \mathrm{ps} . L_{x}=300 \mathrm{~nm}$.

$$
\mathrm{T}_{\text {qa }}^{\mathrm{L}}(\mathrm{meV}) \quad+
$$


$\mathrm{T}^{\mathrm{L}}{ }_{\text {qa }}(\mathrm{meV}) \quad+$


Figure 4.43: The coupling energies between the states situated in the sample and states of the lowest subband in the leads for the first and second bias window ( $B=0.2 \mathrm{~T}$ ).

One the other hand for both bias windows, increasing magnetic field reduces the electron transfer.

Like in our previous section (Modulated currents), the number of
$\mathrm{T}^{\mathrm{L}}{ }_{\text {qa }}(\mathrm{meV})$

$\mathrm{T}_{\mathrm{qa}}^{\mathrm{L}}(\mathrm{meV})$


$$
\mathrm{T}_{\text {qa }}^{\mathrm{L}}(\mathrm{meV}) \quad+
$$


$\mathrm{T}^{\mathrm{L}} \mathrm{qa}^{(\mathrm{meV})}$


Figure 4.44: The coupling tensor between the states $a=2-5$ and states of the lowest subband in the leads for $B=0.2,0.4,0.6,0.8 \mathrm{~T}$ (first bias window). $L_{x}=300 \mathrm{~nm}$.
electrons increases with increasing coupling between the leads and the sample. Here, the parameters for strong coupling are: $g_{0} a_{w}^{3 / 2}=1200$ $\mathrm{meV}, \delta_{1} a_{w}^{2}=0.75$, and $\delta_{2} a_{w}^{2}=1.5$.

We analyze the probability density associated to the five active singleelectron states (number 6-10) of the finite quantum wire (Figure 4.45).

The figures indicates that all the five states have the characteristics of edge states. As the magnetic field increases the Lorentz force squeezes the probability of some states close to the edge of the finite wire. This also happens at the hard-wall ends of the wire, the contact area. This fact explains why the increasing of the coupling through increasing $g_{0}$ should be more effective at high magnetic field. It is evident that the edge states will have different coupling strengths to the leads due to the difference in their finer structure in the contact area. This finer structure in the contact area of the wire induces differential coupling to the states in the different subbands of the leads.

The time-dependent charge in the quantum wire is shown in Figure 4.46.

The charge distribution reflects the geometry of the quantum wire and of the five SESs involved. The selected time moments cover the initial charging cycle plus a part of the next cycle. It is interesting to observe how the electrons are injected at the left contact into the sample traveling along the quantum wire on the upper edge channel, and how they are reflected back at the right contact traveling along the lower channel.


Figure 4.45: The probability density of the single-electron eigenstates of the sample number $6-10$, for $B=1 \mathrm{~T} . L_{x}=300 \mathrm{~nm}$.

$t=14.43 \mathrm{ps}$

$\mathrm{t}=38.0 \mathrm{ps}$



## 4. TIME DEPENDENT TRANSPORT



Figure 4.46: The average spatial charge distribution in the quantum wire for $B=1 \mathrm{~T}$, at different time moments. $g_{0} a_{w}^{3 / 2}=1200 \mathrm{meV}, \delta_{1} a_{w}^{2}=0.75$, and $\delta_{2} a_{w}^{2}=1.5 . L_{x}=300 \mathrm{~nm}$.

### 4.3.3 Coupling strength

Another important aspect in our model is the strength of the lead-sample coupling, the parameters $g_{0}, \delta_{1}$, and $\delta_{2}$.
Our GME implementation is restricted to the lowest order in $H_{T}$, in the kernel of an integro-differential equation, and thus the parameters have to be appropriately selected. In general it is difficult to evaluate whether the coupling strength is sufficiently low.
A necessary (although not sufficient) condition is to obtain positive diagonal elements of the statistical operator, which are the populations of the MES and hence probabilities. Although we always check in our calculations, strictly speaking this condition does not guarantee the validity of the lowest order approximation. So in practice we cannot avoid choosing our parameters in a semi-empirical manner.

To have an idea about the relation between the pumping amplitude and the coupling strength we show in Figure 4.47 three calculations done with three strengths of the coupling, which we consider in relative terms weak, intermediate, and strong.


Figure 4.47: The time dependent total occupation for $B=0 \mathrm{~T}$ and three values of the coupling strength. Weak: $g_{0} a_{w}^{3 / 2}=1408 \mathrm{meV}, \delta_{1} a_{w}^{2}=1.85$, $\delta_{2} a_{w}^{2}=3.7$. Intermediate: $g_{0} a_{w}^{3 / 2}=1408 \mathrm{meV}, \delta_{1} a_{w}^{2}=1.39, \delta_{2} a_{w}^{2}=2.77$. Strong: $g_{0} a_{w}^{3 / 2}=1824 \mathrm{meV}, \delta_{1} a_{w}^{2}=1.39, \delta_{2} a_{w}^{2}=2.77$. The pulse period is $T=60 \mathrm{ps} . L_{x}=300 \mathrm{~nm}$.

## 4. TIME DEPENDENT TRANSPORT

In order to compare with the results obtained in the presence of a magnetic field shown in the next examples, the scaled parameters $g_{0} a_{w}^{3 / 2}$ and $\delta_{1,2} a_{w}^{2}$ are chosen such that the physical values $g_{0}$ and $\delta_{1,2}$ are the same as for $B=0.9 \mathrm{~T}$. The time dependent occupation of the states in the active window is shown for longer times than in the previous figures to indicate better the final periodic regime. It is not surprising to see that the pumping amplitude increases with the coupling strength, since tunneling of electrons becomes more likely.

We already have seen that the increasing of magnetic field reduces the electron transfer if the parameters describing the coupling are scaled. The general situation is more complex. To show that we solve the GME for a fixed magnetic field $B=0.9 \mathrm{~T}$ for three sets of coupling parameters, which we again call (in relative terms) weak, intermediate, and strong coupling, respectively, see Figure 4.48.


Figure 4.48: The time dependent total occupation for $B=0.9 \mathrm{~T}$ and three coupling strength: weak $\left(g_{0} a_{w}^{3 / 2}=926 \mathrm{meV}, \delta_{1} a_{w}^{2}=1.0\right.$, and $\delta_{2} a_{w}^{2}=$ 2.0), intermediate ( $g_{0} a_{w}^{3 / 2}=926 \mathrm{meV}, \delta_{1} a_{w}^{2}=0.75$, and $\delta_{2} a_{w}^{2}=1.5$ ), and strong $\left(g_{0} a_{w}^{3 / 2}=1200 \mathrm{meV}, \delta_{1} a_{w}^{2}=0.75\right.$, and $\left.\delta_{2} a_{w}^{2}=1.5\right)$. The pulse period is $T=60 \mathrm{ps} . L_{x}=300 \mathrm{~nm}$.

The parameters for the weak coupling are the same as in Figure 4.47. For the intermediate coupling we use $g_{0} a_{w}^{3 / 2}=926 \mathrm{meV}, \delta_{1} a_{w}^{2}=0.75$, and $\delta_{2} a_{w}^{2}=1.5$. For the strong coupling $g_{0} a_{w}^{3 / 2}=1200 \mathrm{meV}, \delta_{1} a_{2}^{2}=0.75$,
and $\delta_{2} a_{w}^{2}=1.5$. So, if we now compare the results at $B=0.9 \mathrm{~T}$ with the results at $B=0$ we see quite similar charge amplitudes, but somewhat more sensitive to the coupling strength at $B=0.9 \mathrm{~T}$. For example, at $B=0.9 \mathrm{~T}$ we obtain $Q_{p} \approx 0.4$ electrons at low coupling, $Q_{p} \approx 1.2$ at intermediate coupling, and $Q_{p} \approx 2.4$ at strong coupling. For $B=0$ these numbers are $Q_{p} \approx 0.3,1.2$, and 1.8, as can be read from Figure 4.47. Of course that this is just a particular case.

Another example ( $B=0.4 \mathrm{~T}$ ) demonstrates that in comparison with $B=0$ the electron transfer decreases for all the couplings ( $Q_{p} \approx 0.3,0.85$ and 1.5 , see Figure 4.49). It is not easy to make a comparison between all of these because when we change the magnetic field we get a new energy spectrum and we should change all the time the chemical potentials in the leads. To get an idea about what happens we shall show the average pumped charge as a function of magnetic field (Figure 4.50). For the higher values of the magnetic field the magnetic length is getting smaller than the characteristic length scales of the sample and clear edge states are forming with reduced backscattering.


Figure 4.49: The time dependent total occupation for $B=0.4 \mathrm{~T}$ and three coupling strength: weak $\left(g_{0} a_{w}^{3 / 2}=1241 \mathrm{meV}, \delta_{1} a_{w}^{2}=1.52\right.$, and $\delta_{2} a_{w}^{2}=3.04$, intermediate $\left(g_{0} a_{w}^{3 / 2}=1241 \mathrm{meV}, \delta_{1} a_{w}^{2}=1.14\right.$, and $\delta_{2} a_{w}^{2}=$ 2.28), and strong ( $g_{0} a_{w}^{3 / 2}=1609 \mathrm{meV}, \delta_{1} a_{w}^{2}=1.14$, and $\left.\delta_{2} a_{w}^{2}=2.28\right)$. The pulse period is $T=60 \mathrm{ps} . L_{x}=300 \mathrm{~nm}$.


Figure 4.50: Pumped charge per cycle, vs. magnetic field for strong coupling. The pulse period is $T=60 \mathrm{ps} . L_{x}=300 \mathrm{~nm}$.

## 5

## Summary

In this thesis a time-dependent model for electron transport through a semiconductor system connected to broad leads was investigated using the generalized master equation formalism.

The model presented here is very flexible, in the sense that the parabolic confinement of the system and the leads can be determined independently and the geometry of the central system can be varied by embedding a series of Gaussian potentials in it representing, quantum dots, rings, or antidots.

We describe phenomenologically the coupling between the individual single-electron states in the semi-infinite leads and the continuous states in the finite wire employing a nonlocal overlap of the wave functions from both sides of the contact.

Properties of the model set-up gave us the possibility to study both the transient and the steady state regime. We do this for a system coupled smoothly to the leads at a specific timepoint. We further investigated if the formalism is appropriate to describe modulated currents and turnstile pumping through the central system.

We have observed how quantum point contacts alter the current and slow down the transient processes. We have in addition seen the dynam-

## 5. SUMMARY

ical formation of a broad resonance state in the QPC.
We have investigated under what condition a signal can be propagated through the central system that is weakly coupled to the broad leads. As a continuation we investigated the turnstile operation of the central system. It was not clear at the outset of the research that a formalism built on the generalized quantum master equation could be used for the description of the signal modulation and turnstile operation, but we have found that this is possible, and we have mapped out the physical parameters that are a necessary precondition.

Due to the special state-dependent coupling scheme we introduce in the thesis built on an idea of a general tunneling Hamiltonian the behavior of the contacts in a magnetic field is not uniquely determined in the absence of a microscopic model. We approach this dilemma by proposing two different ways the coupling scheme can depend on the magnetic field. Both schemes display interesting magnetic field effects in the transport, with the subtle difference only to be determined by an experiment or a microscopic model of the contacts.

The numerical accuracy of the results presented in this work has been tested by varying the size of the relevant functional basis and tuning integration and converging schemes.

We did not include the electro-electron interaction as we have only taken the first steps to use the GME formalism for a system with rich geometry without resorting to the Markov approximation. We are dealing with a system with a variable number of electrons where different charging regimes may be of importance depending on the type of coupling between the leads and the system. One has to remember that the coupling to the leads in the many-electron formalism used forces correlation on the electron states of the central system even though we do not include Coulomb interaction between the electrons.

## Appendix A

## Appendices

## A. 1 Derivation of GME

In this appendix we derive the generalized master equation (GME). To simplify the notations we first define the Liouville-von Neumann operator $\mathcal{L}(t)$

$$
\begin{equation*}
\mathcal{L}(t) A=[H(t), A], \tag{A.1}
\end{equation*}
$$

where $A$ is any operator from the Hilbert space and $H(t)$ the Hamiltonian, in principle time dependent. The statistical operator of the total system, which is the sample plus the two leads, $W(t)$, satisfies the Liouville equation (or equation of motion)

$$
\begin{equation*}
i \hbar \frac{d W(t)}{d t}=[H(t), W(t)] \equiv \mathcal{L}(t) W(t) \tag{A.2}
\end{equation*}
$$

The Hamiltonian has the form $H=H_{S}+H_{\text {leads }}+H_{T}$ and thus the Liouville operator can be decomposed in three terms: $\mathcal{L}_{S}=\left[H_{S}, \cdot\right]$, $\mathcal{L}_{\text {leads }}=\left[H_{\text {leads }}, \cdot\right], \mathcal{L}_{T}=\left[H_{T}, \cdot\right]$, such that $\mathcal{L}=\mathcal{L}_{S}+\mathcal{L}_{\text {leads }}+\mathcal{L}_{T}$.

The total statistical operator $W$ includes the distribution of states in the leads, in the sample, and in the connected system, in a combined and complicated manner. In the absence of the contacts, i.e. for isolated leads and sample, it becomes the product of the separate statistical operators.

Assuming the leads and the sample are disconnected at $t \leq 0$ we have

$$
\begin{equation*}
W(t \leq 0)=\rho_{\text {leads }} \rho_{S} \tag{A.3}
\end{equation*}
$$

where $\rho_{\text {leads }}$ and $\rho_{S}$ are statistical operators for the isolated leads and the isolated sample. At $t>0$ the statistical operator for the sample is defined as a mean value of the total statistical operator over the degrees of freedom corresponding to the leads

$$
\begin{equation*}
\rho(t)=\operatorname{Tr}_{l e a d s} W(t), \tag{A.4}
\end{equation*}
$$

having the initial value $\rho(0)=\rho_{S}$ used in Equation (A.3). $\rho(t)$ is called the reduced density operator (RDO).

We define now the projector operator $\mathcal{P}=\rho_{\text {leads }} \operatorname{Tr}_{\text {leads }}$, and thus we can write

$$
\begin{equation*}
\mathcal{P} W(t)=\rho_{\text {leads }} \rho(t) \tag{A.5}
\end{equation*}
$$

and we will also use the complement of $\mathcal{P}$, defined as $\mathcal{Q}=1-\mathcal{P}$. These two operators have the following simple properties

$$
\begin{equation*}
\mathcal{P}^{2}=\mathcal{P}, \quad \mathbb{Q}^{2}=\mathcal{Q}, \quad \mathcal{P} Q=Q \mathcal{P}=0 \tag{A.6}
\end{equation*}
$$

Acting now with both $\mathcal{P}$ and $\mathcal{Q}$ on both sides of Equation (A.2) we can transform this equation into the system of equations

$$
\begin{align*}
& i \hbar \mathcal{P} \dot{W}=\mathcal{P} \mathcal{L} W=\mathcal{P} \mathcal{L}(\mathcal{P}+\mathcal{Q}) W  \tag{A.7}\\
& i \hbar \mathscr{W}=\mathcal{L} W=\mathcal{L} \mathcal{L}(\mathcal{P}+\mathcal{Q}) W
\end{align*}
$$

It is now straightforward to show the following properties

$$
\begin{equation*}
\mathcal{P} \mathcal{L}_{S}=\mathcal{L}_{S} \mathcal{P}, \quad \mathcal{P} \mathcal{L}_{\text {leads }} \mathcal{P}=0, \quad \mathcal{P} \mathcal{L}_{T} \mathcal{P}=0 \tag{A.8}
\end{equation*}
$$

which used in Equations (A.7) lead to

$$
\begin{align*}
i \hbar \mathcal{P} \dot{W} & =\mathcal{L}_{S} \mathcal{P}+\mathcal{P} \mathcal{L}_{T} \mathcal{Q} W  \tag{A.9}\\
i \hbar \mathfrak{W} & =\mathcal{L}_{T} \mathcal{P} W+\left(\mathcal{L}_{S}+\mathcal{L}_{\text {leads }}+\mathcal{L}_{T}\right) \mathcal{Q} W
\end{align*}
$$

## A. 1 Derivation of GME

In order to find the RDO we have to solve the differential system (A.9) where the unknown functions are $\mathcal{P} W$ and $Q W$. At the present stage we need to eliminate the second unknown function $Q W$ to obtain an equation only for the RDO . One possibility is to do iterations: We neglect the term $Q \mathcal{L}_{T} Q W$ on the right side of the second Equation (A.9), we use the resulting solution for $\mathcal{Q} W$ in the first equation, solve it (formally) for $\mathcal{P} W$, return in the second equation, and so on. This procedure leads to a formal solution for $\mathcal{P} W$ written as a time-ordered product of exponentials of $\mathcal{L}_{T}$. Here we want to obtain the solution for a relatively weak strength of the contacts. To do that let's observe that in the limit $H_{T} \rightarrow 0$ the sample and the leads become disconnected and according to Equations (A.3-A.5) we get

$$
\begin{equation*}
\lim _{H_{T} \rightarrow 0} \mathcal{P} W(t)=\rho_{\text {leads }} \rho_{S}=W(0) \tag{A.10}
\end{equation*}
$$

This simply means that in the low-coupling limit the system evolves very slowly, or $\mathcal{P} \rightarrow 1$, or $Q \rightarrow 0$. Thus, for finite, but sufficiently weak coupling we can consider $Q$ a "small" parameter. Therefore, in this situation we can say that $Q \mathcal{L}_{T} \ll \mathcal{L}_{S}+\mathcal{L}_{\text {leads }}$ and the second Equation (A.7) becomes

$$
\begin{equation*}
i \hbar Q \dot{W}=\mathcal{L}_{T} \mathcal{P} W+\left(\mathcal{L}_{S}+\mathcal{L}_{\text {leads }}\right) Q W \tag{A.11}
\end{equation*}
$$

We see in Equation (A.11) a simple first-order linear differential equation for $\mathcal{Q} W(t)$ with the inhomogeneous term $\mathcal{L}_{T} \mathcal{P} W(t)$. To find the solution we first write the general solution of the homogeneous equation, which has the form

$$
\begin{equation*}
R(t)=e^{\left(H_{S}+H_{\text {leads }}\right) t / i \hbar} B e^{-\left(H_{S}+H_{\text {leads }}\right) t / i \hbar} \tag{A.12}
\end{equation*}
$$

where $B$ is a time independent (constant) operator. We now need to find a particular solution of the inhomogeneous Equation (A.12), which can be done with the so-called method of variation of constants. $B$ is forced

## A. APPENDICES

now to be time dependent, and $R(t)$ is inserted in Equation (A.11). The resulting differential equation for $B(t)$ can be easily solved and we obtain

$$
\begin{equation*}
B(t)=\int_{0}^{t} d s e^{-\left(H_{S}+H_{\text {leads }}\right) s / i \hbar}\left(\frac{1}{i \hbar} \mathcal{L}_{T} \mathcal{P} W(s)\right) e^{\left(H_{S}+H_{\text {leads }}\right) s / i \hbar} \tag{A.13}
\end{equation*}
$$

We used the initial condition $Q W(0)=0$ which implies $B(0)=0$. So now the formal solution for of Equation (A.11) is

$$
\begin{equation*}
Q W(t)=\frac{1}{i \hbar} \int_{0}^{t} d s U(t-s) \mathcal{L}_{T} \mathcal{P} W(s) U^{\dagger}(t-s) \tag{A.14}
\end{equation*}
$$

where we have used the time evolution operator of the disconnected system $U(t)=e^{\left(H_{S}+H_{\text {leads }}\right) t / i \hbar}$. Now we go back into the first Equation (A.9) where we substitute $2 W(t)$ and we obtain

$$
\begin{equation*}
\mathcal{P} \dot{W}(t)=\frac{1}{i \hbar} \mathcal{L}_{S} \mathcal{P} W(t)+\frac{1}{(i \hbar)^{2}} \mathcal{P} \mathcal{L}_{T} \int_{0}^{t} d s U(t-s) \mathcal{L}_{T} \mathcal{P} W(s) U^{\dagger}(t-s) \tag{A.15}
\end{equation*}
$$

which is the generalized master equation (GME). Using the definition of the projector $\mathcal{P}$ and of the Liouville operators we can write it as:

$$
\begin{align*}
\dot{\rho}(t) & =\frac{1}{i \hbar}\left[H_{S}, \rho(t)\right]  \tag{A.16}\\
& +\frac{1}{(i \hbar)^{2}} \operatorname{Tr}\left[H_{T}(t), \int_{0}^{t} d s U(t-s)\left[H_{T}(s), \rho_{l e a d s} \rho(t)\right] U^{\dagger}(t-s)\right]
\end{align*}
$$

The GME is an integro-differential equation which in the present form is second order in the transfer Hamiltonian $H_{T}$ in its kernel. But the solution can actually be seen as power series in $H_{T}^{2}$. So it is not necessarily valid only in the lowest (second) order of the coupling strength.

We now use the explicit form of the transfer Hamiltonian $H_{T}$ given in Equation (3.6) defined with the creation and annihilation operators in the leads, $c_{q l}^{\dagger}, c_{q l}$ and in the sample, $d_{a}^{\dagger}, d_{a}$. We then calculate the internal commutator combined with the evolution operator,

$$
\begin{equation*}
U(t-s)\left[H_{T}(s), \rho_{\text {leads }} \rho(t)\right] U^{\dagger}(t-s) \tag{A.17}
\end{equation*}
$$

## A. 1 Derivation of GME

using the commutation of the field operators in the leads with those in the sample. The (fermionic) field operators in the leads satisfy the anticommutation rules $\left\{c_{q l}, c_{q^{\prime} l}\right\}=\left\{c_{q l}^{\dagger}, c_{q^{\prime} l}^{\dagger}\right\}=0,\left\{c_{q l}, c_{q^{\prime} l}^{\dagger}\right\}=\delta_{q q^{\prime}}$. We also use the relation

$$
e^{H_{\text {leads }} t / i \hbar} c_{q l} e^{-H_{\text {leads }} t / i \hbar}=c_{q l} e^{-\epsilon_{q}^{l} t / i \hbar}
$$

and the corresponding Hermitian conjugate (42). The explicit form of the operator (17) is long and we will not write it here, but it becomes simpler after we carry on the trace ( Tr ) in Equation (A.16). To do that we introduce the Fermi functions in the leads as

$$
\begin{aligned}
\operatorname{Tr}\left(c_{q^{\prime} l}^{\dagger} c_{q l} \rho_{\text {leads }}\right) & =\delta_{q q^{\prime}} f_{l} \\
\operatorname{Tr}\left(c_{q l} c_{q^{\prime} l}^{\dagger} \rho_{\text {leads }}\right) & =\delta_{q q^{\prime}}\left(1-f_{l}\right)
\end{aligned}
$$

In the end the GME takes the form shown in the main text, in Equations (3.18-3.19)

We solve the GME numerically by discretizing the time, using the Crank-Nicolson method. For each time step $t_{n}$ we find $\rho\left(t_{n}\right)$ by iterations.

## A. 2 Matrix elements for the Potential

In this section we will show the analytical calculations for the matrix elements of the potential describing an embedded subsystem in the quantum wire. The subsystem is represented by a combination of Gauss potentials of the form

$$
\begin{equation*}
W_{i}(x, y)=V_{i} e^{\left[-\beta_{x, i}\left(x-x_{i}\right)\right]^{2}-\left[\beta_{y, i}\left(y-y_{i}\right)\right]^{2}} \tag{A.18}
\end{equation*}
$$

where $V_{i}$ is the strength of the potential, while $\left(x_{i}, y_{i}\right)$ and $\beta_{(x, y), i}$ control the range of the potential. $W_{i}(x, y)$ is separable and thus we can consider the integrals for the matrix element in our SES basis separately.

The matrix elements for the $x$ part are

$$
\begin{equation*}
V_{i ; m, m^{\prime}}=\int_{-L_{x} / 2}^{L_{x} / 2} d x \psi_{m}^{*}(x) W_{i}(x, y) \psi_{m^{\prime}}(x) \tag{A.19}
\end{equation*}
$$

where $\psi_{m}(x)$ is the basis function in the $x$ direction.

$$
\begin{equation*}
\psi_{m}(x)=\sqrt{\frac{2}{L_{x}}} \cos \left(\frac{m \pi x}{L_{x}}\right), \quad \quad m=o d d \tag{A.20}
\end{equation*}
$$

and

$$
\begin{equation*}
\psi_{m^{\prime}}(x)=\sqrt{\frac{2}{L_{x}}} \sin \left(\frac{m^{\prime} \pi x}{L_{x}}\right), \quad m^{\prime}=\text { even } \tag{A.21}
\end{equation*}
$$

From Equations (A.20-A.21) we see that if $m+m^{\prime}=1$, then $V_{i ; m, m^{\prime}}(y)$ $=0$.
On the other hand, if $m+m^{\prime}=0$, then

## A. 2 Matrix elements for the Potential

$$
\begin{align*}
V_{i ; m, m^{\prime}} & =\frac{2}{L_{x}} \int_{-L_{x} / 2}^{L_{x} / 2} d x \sin \left(\frac{m \pi x}{L_{x}}\right) \sin \left(\frac{m^{\prime} \pi x}{L_{x}}\right) e^{-\left[\beta_{x, i}\left(x-x_{i}\right)\right]^{2}} \\
& =\frac{2}{\pi} \int_{0}^{\pi / 2} d x\left[\cos \left(m-m^{\prime}\right) x-\cos \left(m-m^{\prime}\right) x\right] e^{-\left[\alpha\left(x-x_{i}\right)\right]^{2}} . \tag{A.22}
\end{align*}
$$

or, if $m+m^{\prime}=2$, we have

$$
\begin{align*}
V_{i ; m, m^{\prime}} & =\frac{2}{L_{x}} \int_{-L_{x} / 2}^{L_{x} / 2} d x \cos \left(\frac{m \pi x}{L_{x}}\right) \cos \left(\frac{m^{\prime} \pi x}{L_{x}}\right) e^{-\left[\beta_{x, i}\left(x-x_{i}\right)\right]^{2}} \\
& =\frac{2}{\pi} \int_{0}^{\pi / 2} d x\left[\cos \left(m-m^{\prime}\right) x-\cos \left(m+m^{\prime}\right) x\right] e^{-\left[\alpha\left(x-x_{i}\right)\right]^{2}} \tag{A.23}
\end{align*}
$$

where $\alpha=\beta_{x, i} L_{x} / \pi$.
Then the first (or the second) expression becomes

$$
\begin{align*}
\int_{0}^{\pi / 2} d x \cos (Z x) e^{-\left[\alpha\left(x-x_{i}\right)\right]^{2}} & =\frac{1}{2} \int_{0}^{\pi / 2} d x\left(e^{i Z x}+e^{-i Z x}\right) e^{-\left[\alpha\left(x-x_{i}\right)\right]^{2}} \\
& =\frac{\sqrt{\pi}}{2 \alpha} e^{-Z^{2} / 4 \alpha^{2}}\left[\Phi\left(\frac{\alpha \pi}{2}-i \frac{Z}{2 \alpha}\right)+\Phi\left(\frac{\alpha \pi}{2}+i \frac{Z}{2 \alpha}\right)\right] \\
& =\frac{\sqrt{\pi}}{2 \alpha} e^{-Z^{2} / 4 \alpha^{2}} \Re\left[\Phi\left(\frac{\alpha \pi}{2}+i \frac{Z}{2 \alpha}\right)\right] \tag{A.24}
\end{align*}
$$

where $\Phi$ is the error function.
We solve the integral by using Equation (3.321.2) on page 354 in (41). By combining Equations (A.22-A.23-A.24) we get

## A. APPENDICES

$$
\begin{align*}
V_{i ; m, m^{\prime}} & =\frac{1}{\alpha \sqrt{\pi}} e^{-\left(m-m^{\prime}\right)^{2} / 4 \alpha^{2}} \Re\left[\Phi\left(\frac{\left(m-m^{\prime}\right) i+\pi \alpha^{2}}{2 \alpha}\right)\right] \\
& +(-1)^{n+1} \frac{1}{\alpha \sqrt{\pi}} e^{-\left(m+m^{\prime}\right)^{2} / 4 \alpha^{2}} \Re\left[\Phi\left(\frac{\left(m+m^{\prime}\right) i+\pi \alpha^{2}}{2 \alpha}\right)\right] \tag{A.25}
\end{align*}
$$

The matrix elements for the $y$ part are

$$
\begin{equation*}
V_{i ; n, n^{\prime}}=\int_{-\infty}^{\infty} d y \psi_{n}^{*}(y) W_{i}(x, y) \psi_{n^{\prime}}(y) \tag{A.26}
\end{equation*}
$$

where $\psi_{n}(y)$ is the wave functions of the subbands for a parabolic confinement

$$
\begin{equation*}
\psi_{n}(y)=\frac{e^{-\frac{y^{2}}{2 a_{w}^{2}}}}{\sqrt{2^{n} \sqrt{\pi} n!a_{w}}} H_{n}\left(\frac{y}{a_{w}}\right) \tag{A.27}
\end{equation*}
$$

The embedded subsystem or Gauss potential is given by Equation (A.18). We have

$$
\begin{equation*}
V_{i ; n, n^{\prime}}=\frac{V_{i}}{\sqrt{2^{n+n^{\prime}} n!n^{\prime}!\pi}} \int_{-\infty}^{\infty} d \bar{y} e^{-\beta_{y, i}^{2} a_{w}^{2}\left(\bar{y}-\bar{y}_{i}\right)^{2}-\bar{y}^{2}} H_{n}(\bar{y}) H_{n^{\prime}}(\bar{y}) \tag{A.28}
\end{equation*}
$$

In the above equation we have used the following notation: $\bar{y}=\frac{y}{a_{w}}$ and also we shall use $\bar{\beta}=\beta_{y, i}^{2} a_{w}^{2}$. The exponent in the integral is

$$
\begin{equation*}
-\bar{\beta}\left(\bar{y}-\bar{y}_{i}\right)^{2}-\bar{y}^{2}=-\left[(\sqrt{1+\bar{\beta}}) \bar{y}-\frac{\bar{\beta} \bar{y}_{i}}{(\sqrt{1+\bar{\beta}})}\right]^{2}-\frac{\bar{\beta} \bar{y}_{i}^{2}}{1+\bar{\beta}} .( \tag{A.29}
\end{equation*}
$$

Using this relation and the notation: $z=\sqrt{1+\bar{\beta}} \bar{y}$ we get

## A. 2 Matrix elements for the Potential

$$
\begin{align*}
& V_{i ; n, n^{\prime}}=\frac{V_{i}}{\sqrt{2^{n+n^{\prime}} n!n^{\prime}!\pi}} \frac{e^{-\frac{\bar{\beta} y_{i}^{2}}{1+\beta}}}{\sqrt{1+\bar{\beta}}} \\
& \quad \times \int_{-\infty}^{\infty} d z e^{-\left(z-\frac{\bar{\beta} y_{i}}{\sqrt{1+\bar{\beta}}}\right)^{2}} H_{n}\left[\frac{z}{\sqrt{1+\bar{\beta}}}\right] H_{n^{\prime}}\left[\frac{z}{\sqrt{1+\bar{\beta}}}\right] . \tag{A.30}
\end{align*}
$$

By using Equation (7.374.9) on page 843 in (41) we obtain

$$
\begin{align*}
& V_{i ; n, n^{\prime}}=\frac{V_{i}}{\sqrt{2^{n+n^{\prime}} n!n^{\prime}!}} \frac{e^{-\frac{\beta_{y, i}^{2} a_{w}^{2} y_{i}^{2}}{1+\beta_{y, i}^{2} a_{w}^{2}}}}{\sqrt{1+\beta_{y, i}^{2} a_{w}^{2}}} \\
& \quad \times \sum_{k=0}^{\min \left(n, n^{\prime}\right)} 2^{k} k!\binom{n}{k}\binom{n^{\prime}}{k}\left(\frac{\beta_{y, i}^{2} a_{w}^{2}}{1+\beta_{y, i}^{2} a_{w}^{2}}\right)^{\frac{n+n^{\prime}}{2}-k} H_{n+n^{\prime}-2 k}\left[\frac{\sqrt{\beta_{y, i}^{2} a_{w}^{2}} y_{i}}{\sqrt{1+\beta_{y, i}^{2} a_{w}^{2}}}\right] . \tag{A.31}
\end{align*}
$$

## A. 3 Semiinfinite wire in a magnetic field

For the semi-infinite leads with the previously introduced confinement parameters, we can use the same basis functions for the $y$ direction, but for the $x$ direction we use

$$
\begin{equation*}
\psi_{q}(x)=\frac{1}{\sqrt{2 \pi}} \sin \left[q\left(x \pm L_{x} / 2\right)\right] \tag{A.32}
\end{equation*}
$$

with "+" in the left lead and " - " in the right lead.
We need to solve

$$
\begin{equation*}
H_{L, R}(B)\left|p n_{y}\right\rangle=E_{p n_{y}}\left|p n_{y}\right\rangle \tag{A.33}
\end{equation*}
$$

and use the expansion

$$
\begin{equation*}
\left|p n_{y}\right\rangle=\sum_{n_{y}^{\prime}} \int d q C^{n_{y} n_{y}^{\prime}}(p, q)\left|q n_{y}^{\prime}\right\rangle \tag{A.34}
\end{equation*}
$$

obtaining

$$
\begin{equation*}
E_{p m_{y}} C^{n_{y} m_{y}}(q, p)=\sum_{n_{y}^{\prime}} \int d k\left\langle q n_{y}\right| H_{L, R}(B)\left|k n_{y}^{\prime}\right\rangle C^{n_{y}^{\prime} m_{y}}(k, p) \tag{A.35}
\end{equation*}
$$

By using that

$$
\begin{align*}
& \left\langle q n_{y}\right| H_{L, R}(B)\left|k n_{y}^{\prime}\right\rangle=\delta_{n_{y} n_{y}^{\prime}} \delta(q-k) E_{q n_{y}}^{0}+ \\
& \left\{\sqrt{\frac{n_{y}^{\prime}}{2}} \delta_{n_{y}, n_{y-1}^{\prime}}+\sqrt{\frac{n_{y+1}^{\prime}}{2}} \delta_{n_{y}, n_{y+1}^{\prime}}\right\} \hbar \omega_{c} a_{w} I_{q k} \tag{A.36}
\end{align*}
$$

## A. 3 Semiinfinite wire in a magnetic field

where $I_{q k}=-\frac{i q p}{2 \pi} \frac{\mathcal{P}}{q^{2}-p^{2}}$,
and simplifying the notations by defining

$$
\begin{equation*}
\bar{Y}_{n_{y}, n_{y}^{\prime}}=\left\{\sqrt{\frac{n_{y}^{\prime}}{2}} \delta_{n_{y}, n_{y-1}^{\prime}}+\sqrt{\frac{n_{y+1}^{\prime}}{2}} \delta_{n_{y}, n_{y+1}^{\prime}}\right\} \tag{A.37}
\end{equation*}
$$

we can rewrite Equation (A.35) as
$E_{p m_{y}} C^{n_{y} m_{y}}(q, p)=\sum_{n_{y}^{\prime}} \int d k\left\{\delta_{n_{y} n_{y}^{\prime}} \delta(q-k) E_{q n_{y}}^{0}+\hbar \omega_{c} a_{w} I_{q k}\right\} C^{n_{y}^{\prime} m_{y}}(k, p)$.

This eigenvalue problem is not convenient for numerical evaluation, so we try an analytical integration of the second term, where $\mathcal{P}$ denotes the principal value

$$
\begin{equation*}
\int_{0}^{\infty} d k \frac{\mathcal{P} k}{q^{2}-k^{2}} C^{n_{y}^{\prime} m_{y}}(k, p)=\frac{1}{2} \int_{-\infty}^{\infty} d k \frac{\mathcal{P}|k|}{q^{2}-k^{2}} C^{n_{y}^{\prime} m_{y}}(|k|, p) \tag{A.39}
\end{equation*}
$$

The integral can be done in the complex plane as, see Figure (A.1).

$$
\begin{equation*}
\frac{1}{2} \int_{-\infty}^{\infty} d k \frac{\mathcal{P}|k|}{q^{2}-k^{2}} C^{n_{y}^{\prime} m_{y}}(|k|, p)=I_{c}-i \pi\{\operatorname{Res} F(q)-\operatorname{Res} F(-q)\} \tag{A.40}
\end{equation*}
$$

where

$$
\begin{equation*}
I_{c}=\frac{i \pi}{2} C^{n_{y}^{\prime} m_{y}}(q, p) \quad \operatorname{Res} F(q)=\frac{|q| C^{n_{y}^{\prime} m_{y}}(q, p)}{2 q} \tag{A.41}
\end{equation*}
$$

By making the substitution of Equations (A.40), (A.41) in (A.38) we get

$$
\begin{equation*}
E_{p m_{y}} C^{n_{y} m_{y}}(q, p)=\sum_{n_{y}^{\prime}}\left\{\delta_{n_{y} n_{y}^{\prime}} E_{q n_{y}^{\prime}}^{0}-\frac{\hbar \omega_{c} a_{w}}{4} q \bar{Y}_{n_{y}, n_{y}^{\prime}}\right\} C^{n_{y}^{\prime} m_{y}}(q, p) \tag{A.42}
\end{equation*}
$$

The interpretation is that for each $q$ we only have to diagonalize the $n^{\max } \times n^{\text {max }}$-matrix where $n^{\max }$ is the maximum number of subbands in the basis. In the contour integration we have assumed that no bound states are formed in the semiinfinite leads.


Figure A.1: The contour for evaluation of the integral (A.39) in the complex plane.

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