

Prediction of a realistic quantum logic gate using the contact block reduction method

M Sabathil¹, D Mamaluy² and P Vogl¹

¹ Walter Schottky Institut, Technische Universität München, Am Coulombwall 3, 85748 Garching, Germany

² Department of Electrical Engineering, Arizona State University, Tempe, AZ 85287-5706, USA

E-mail: sabathil@wsi.tum.de

Received 26 July 2003

Published 3 March 2004

Online at stacks.iop.org/SST/19/S137 (DOI: 10.1088/0268-1242/19/4/048)

Abstract

We present a theoretical study of the realization of a quantum logic gate based on a laterally structured high mobility GaAs/AlGaAs 2DEG. The I – V characteristics exhibit a pronounced switching behaviour which demonstrates that quantum logic gates can be fabricated and operated experimentally. The calculations have been performed with the recently developed contact block reduction method. We show that this method can be readily extended to multi-band $\mathbf{k} \cdot \mathbf{p}$ -Hamiltonians while retaining its efficiency.

1. Introduction

In a semiconductor heterostructure, a single qubit may be realized by electrons propagating ballistically within two adjacent quantum wires [1, 2]. The $|0\rangle$ and $|1\rangle$ basis states are then represented by an electron fully localized in one of the wires. Based on this concept, single- and two-qubit gates have been proposed [1, 2]. In this work we predict a realistic single qubit switch that operates via gate-controlled interference between a pair of adjacent quantum wires. The interference is induced by narrow windows in the barrier region between the wires that act as beam splitters, allowing the 0 and 1 states to interfere. Additional gates are needed to control the phase shifts within one of the wires. Here, we propose a concrete solid-state realization of a Mach–Zehnder interferometer (figure 1, inset) based on an AlGaAs/GaAs three-dimensional (3D) nanostructure. The interference-induced switching can be observed via the ballistic current.

2. Logic gate with single band CBR method

The active region of our quantum logic device is an AlGaAs/GaAs high mobility two-dimensional electron gas (2DEG) with several top gates that produce the required lateral confinement. The bottom of figure 1 shows a cross section through the structure that is grown on an Al_{0.3}Ga_{0.7}As substrate

with a 10 nm wide n⁺ doping ($5 \times 10^{18} \text{ cm}^{-3}$) layer followed by a 30 nm intrinsic buffer layer. The 2DEG is confined in a 10 nm GaAs quantum well followed by another 20 nm Al_{0.3}Ga_{0.7}As buffer. A second n⁺ doping region of 10 nm width ($1 \times 10^{18} \text{ cm}^{-3}$) accounts for the filling of the quantum well. Finally, there is a Schottky contact at the top of the structure. None of the lateral scales lies below 50 nm. This electrostatic confinement via the gates offers sufficient potential variation in order to steer the device.

The quantum transport through the device has been calculated in two steps. Firstly, the equilibrium potential profile of the three-dimensional structure including the gate electrodes has been calculated self-consistently, using our device simulator **nextnano**³ [3]. This amounts to solving the fully 3D one-band Schrödinger equation together with the 3D Poisson equation self-consistently. Secondly, the ballistic transmission through the device is computed with the contact block reduction (CBR) method [4] which yields the current via the Landauer formula. The results in figure 2 show that the stationary current can indeed be switched from a non-inverting to an inverting state. The former corresponds to a unity qubit transformation, whereas the latter corresponds to a flip of the qubit. The phase shifting gate P controls the flow from the left leads to the right leads. For a gate voltage of -15 mV , figure 2 shows a large current flow between the leads In $|1\rangle$ to Out $|1\rangle$ and In $|0\rangle$ to Out $|0\rangle$, respectively, which corresponds

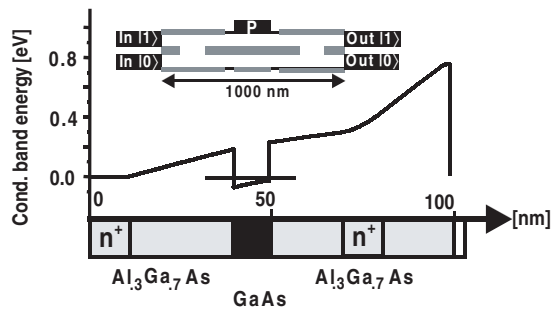


Figure 1. Top inset: schematic top view of the proposed solid-state Mach-Zehnder interferometer. The grey areas are barriers introduced via top gates. The P-gate acts as a phase shifter for the upper channel. The two windows in the middle barrier act as beam splitters for the electrons in the channel. Bottom: vertical cross section through the structure. Middle: conduction band profile in eV in the growth direction. Details are described in the text.

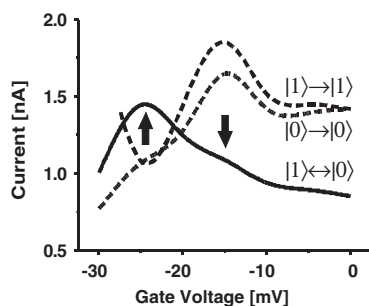


Figure 2. Source-drain current through the interferometer as a function of phase-shifting gate voltage. The full line marks the current between the $|0\rangle$ and $|1\rangle$ leads, dashed lines label the current between the $|0\rangle$ to $|0\rangle$ or $|1\rangle$ to $|1\rangle$ leads, respectively. The arrows indicate the voltages of maximal switching.

to a current from $0 \rightarrow 0$ and $1 \rightarrow 1$. For a gate voltage of -25 mV, by contrast, the current flows dominantly from $0 \rightarrow 1$ and $1 \rightarrow 0$ which corresponds to an inversion. The efficiency is about 30% for the chosen temperature of 200 mK and an applied source-drain bias of 0.05 mV.

3. Multiband CBR method and results

The calculations presented in the first part of this work showed that the CBR method is an efficient scheme to compute the ballistic transmission coefficient through a 3D device using a one-band Hamiltonian. In the second part of this work, we generalize this method to multi-band $\mathbf{k} \cdot \mathbf{p}$ -Hamiltonian systems in order to deal with p-type devices, narrow-band materials and molecular electronic systems. The main idea of the CBR method is to consider separately the problem of a closed system that is described by an Hermitian Hamiltonian \mathbf{H}^0 , and the open, current-carrying system that is described by a non-Hermitian Hamiltonian $\mathbf{H} = \mathbf{H}^0 + \Sigma$ where Σ represents the self-energy due to the coupling to the attached leads. As Σ is nonzero only at the contact regions, one can reformulate the scattering problem in such a way that the transmission coefficient $T(E)$ is obtained through the determination of a small subset of eigenvalues of \mathbf{H}^0 and the repeated solution (i.e. for each energy E) of a small linear system of equations of size Σ . The generalization of this method to multi-band

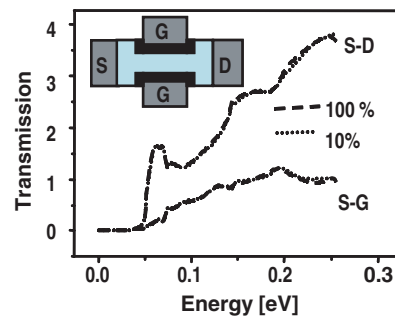


Figure 3. Transmission as a function of energy from source to drain (S-D) and source to gate (S-G) of a double gate SiGe p-MOSFET model. The dashed lines show the results for all eigenvectors and the dotted lines show the transmission for a reduced set of only 10% of all eigenvectors.

Hamiltonians involves two aspects. Firstly, the calculation of the lead modes requires the solution of a non-Hermitian eigenvalue [5] problem for each energy in $T(E)$. Its size is determined by the number of grid points in the contacts and the number of bands included. This procedure increases the total computing time roughly proportional to the number of bands relative to the one-band case. Secondly, one needs to determine boundary conditions for the closed system Hamiltonian \mathbf{H}^0 that mimic open boundary conditions but leave the system Hamiltonian Hermitian. This can be achieved by adding the Hermitian part of the zero energy limit of the self-energy to \mathbf{H}^0 .

To demonstrate the efficiency of the CBR method in the multi-band case, we have calculated the transmission through a 2D 20×10 nm SiGe double gate p-MOSFET model (see the inset of figure 3). We used a four band $\mathbf{k} \cdot \mathbf{p}$ Hamiltonian that includes light and heavy hole bands. All biases are set to zero and the channel potential is also set to zero, except for the barrier regions (shown in black in the inset) that are taken to be 0.4 eV. The $\mathbf{k} \cdot \mathbf{p}$ parameters are used for p-Ge throughout the whole device. Figure 3 shows the transmission function between the source and the drain (S-D) as well as between the source and the gate (S-G). The results show that the method is converged already when only 10% of all eigenvectors are taken into account. Thus, the efficiency of the CBR method is not limited to one-band models and can be successfully applied to multi-band situations.

Acknowledgments

Financial support by the Deutsche Forschungsgemeinschaft and by the Office of Naval Research under contract no N00014-01-1-0242 is gratefully acknowledged.

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