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Design and computer simulations of the nanodevices to applications in quantum computing

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Abstract

In this thesis we propose several nanodevices that exploit the self-focusing effect of a hole or an electron wave function as well as the spin-orbit interaction in order to realize various operations on an electron and hole spin confined in semiconductor gated nanodevices without application of a magnetic field. The proposed devices fulfill the criteria for the physical implementation of quantum computation and are promising candidates for basic building blocks of an all-electrically controlled spin based scalable semiconductor solid state quantum computer architecture. The thesis consists of six chapters: chapter (1) contains the introduction in which we give a short historic overview of the ideas which lay behind quantum computation, list most popular proposals for the physical implementation of quantum computers, describe the spin based proposals for the realization of quantum computers and finally give a short overview of the proposed devices. The summary of the articles which were published as a result of the research done within this PhD are included in chapter (2). The articles are attached in chapters (3)-(6). In chapter (3) nanodevices for single electron spin initialization and read out are proposed that exploit the Dresselhaus spin-orbit interaction. Chapter (4) contains the description of improved nanodevices of the previous chapter (3) which now are capable to realize high fidelity spin accumulation of single electrons and nondestructive single electron spin read out, both without application of a magnetic field, while this time the Rashba spin-orbit interaction is employed. In the next chapter (5) we propose a method for the coherent manipulation of single heavy-hole spin qubits, based on the hole motion-induced heavy-hole spin rotations in the presence of the Dresselhaus spin-orbit interaction and present a nanodevice which can act as a single quantum logic NOT gate. Nanodevices which can realize several all-electrically controlled single quantum logic gates (i.e. Pauli X, Y and Z) on heavy-hole spin qubits based on the method from chapter (5) are proposed in the last chapter (6). Furthermore, in chapter (6) “a combo” nanodevice which can realize an arbitrary sequence of single quantum logic gates on heavy-hole spin qubits is proposed as well as a fragment of a scalable quantum computer architecture containing four qubits. At the and the summary of the thesis is included.

Streszczenie

Niniejszej praca dotyczy projektowania i symuluacji działania nanourządzeń wykonujących kwantowe operacje logiczne na spinie elektronu (dziury) uwięzionego w półprzewodnikowej nanostrukturze bez konieczności stosowania pola magnetycznego. Wykorzystany jest w nich efekt samoogniskowania funkcji falowej elektronu lub dziury oraz oddziaływanie spin-orbita. Zaproponowane nanourządzenia spełniają kryteria fizycznej implementacji komputerów kwantowych i są bardzo obiecującymi kandydatami na podstawowe elementy skalowalnej architektury komputera kwantowego opartej o nanostruktury półprzewodnikowe, ponieważ qubit spinowy jest kontrolowany wyłącznie za pomocą niewielkich napięć przykładanych do elektrod. Praca składa się z sześciu rozdziałów: w rozdziale (1) zawarty jest wstęp obejmujący krótki rys historyczny dotyczący idei obliczeń kwantowych, lista najpopularniejszych propozycji fizycznej realizacji komputerów kwantowych ze szczególnym uwzględnieniem rozwiązań wykorzystujących jako kubit spin elektronu uwięzionego w półprzewodnikowych nanostrukturach. Rozdział kończy się krótkim opisem zaproponowanych w pracy nowych nanourządzeń. Podsumowanie artykułów zawierających wyniki uzyskane podczas realizacji doktoratu zawarte są w rozdziale (2). Publikacje tworzące dysertację zamieszczone są w rozdziałach kolejno od (3) do (6). W rozdziale (3) dyskutowane są nanourządzenia służące do ustawiania oraz do odczytu spinu pojedynczego elektronu. Rozdział (4) zawiera propozycję i opis nanourzadzeń zdolnych do ustawiania i nieniszczącego odczytu stanu spinowego elektronu bez konieczności stosowania pola magnetycznego. Są one w dużym stopniu ulepszone w stosunku do nanourzadzeń zaproponowanych w rozdziale (3). W kolejnym rozdziale (5) przedstawiamy metodę wykonywania koherentnych operacji na kubicie realizowanym przez stan spinowy dziury ciężkiej. Tego typu rozwiązanie jest korzystne ponieważ spin dziury ciężkiej w porównaniu do spinu elektronu cechuje się znacznie dłuższym czasem koherencji. Proponujemy nanourządzenie wykonujące na spinie dziury kwantową operację logiczną NOT. W ostatnim rozdziale (6) przedstawiona jest propozycja nanourzadzeń, które są w stanie wykonywać, różne kwantowe operacje logiczne (np. bramki Pauligo X, Y i Z) na pojedynczym dziurowym kubicie spinowym. W rozdziale (6) zaproponowane jest ponadto nanourządzenie "combo" zdolne do wykonywania dowolnej sekwencji jednokubitowych operacji logicznych oraz fragment skalowalnej architektury (zawierającej cztery kubity) składającej się z takich nanourządzeń. Na końcu pracy znajduje się podsumowanie.

Abstract

In deze thesis stellen we een aantal nanodevices voor die gebruik maken van het zelf-focusing effect van een holte of elektron en van de spin-baan interactive om verschillende logische operaties te implementeren op de spin van een elektron en holte in halfgeleider nanodevices met gates en zonder een uitwendig aangelegd magneetveld. De voorgestelde devices voldoen aan de criteria voor de fysische implementatie van kwantumcomputatie en zijn veelbelovende bouwstenen voor een volledig elektrostatisch gecontroleerde spin gebaseerde schaalbare halfgeleider kwantumarchitectuur. De thesis omvat 6 hoofdstukken. Hoofdstuk (1) geeft een inleiding met een kort historisch overzicht met de ideeën achter kwantumcomputatie. Daarnaast bespreekt het de meest populaire voorstellen voor de fysische implementatie van een kwantumcomputer, de spin gebaseerde voorstellen in het bijzonder. Tot slot wordt een kort overzicht gegeven van de devices die voorgesteld worden in deze thesis. Een samenvatting van de artikels die gepubliceerd werden voortvloeiende uit het onderzoek dat verricht werd in dit doctoraat wordt gegeven in hoofdstuk 2. De artikels zijn toegevoegd als hoofdstukken (3) tot (6). In hoofdstuk (3) worden de nanodevices voor de initialisatie en uitlezing van een enkele elektron spin voorgesteld. Deze devices maken gebruik van de Dresselhaus spin-baan interactie.In hoofdstuk (4) komen verbeterde versies van deze nanodevices aan bod komen die het mogelijk maken om de spin van een elektron niet-destructief uit te lezen, en dit zonder gebruik te maken van een uitwendig aangelegd magneetveld. Hierbij wordt gebruik gemaakt van de Rashba spin-baan koppeling. In het volgende hoofdstuk (5) stellen we een methode voor voor de coherente manipulatie van een enkele heavy-hole qubit, gebaseerd op de beweging van de holte door geïnduceerde holte spin rotaties door de aanwezigheid van de Dresselhaus spin-baan interactie. Hier beschrijven we een nanodevice dat een kwantum logische NOT gate realiseert. Nanodevices voor verschillende volledig elektrostatisch gecontroleerde kwantum logische operaties(i.e. Pauli X,Y en Z) op heavy-hole spin qubits, gebruik makende van de methode van hoofdstuk (5), worden voorgesteld in hoofdstuk (6). Bovendien wordt in hoofdstuk (6) ook een ”combo” device voorgesteld dat in staat is om een willekeurige sequentie van kwantum logische operaties uit te voeren op een heavy-hole qubit, en een fragment van een schaalbare kwantumcomputerarchitectuur met vier qubits. Tot slot volgt een samenvatting.

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About the thesis

The present dissertation consists of monothematic articles in which we propose several nanodevices that exploit the soliton effect of a hole or an electron wave function as well as the spin-orbit interaction in order to realize all-electrically controlled operations on electron and a hole spin qubits confined in gated semiconductor nanostructures for quantum computing applications. The dissertation is composed of the following articles:

A1 P. Szumniak, S. Bednarek, P. Grynkiewicz, B. Szafran *Nanodevice for High Precision Readout of Electron Spin*,
Acta Physica Polonica A 119, 651 (2011).

A2 S. Bednarek, P.Szumniak, and B. Szafran *Spin accumulation and spin read out without magnetic field*,
Phys. Rev. B 82, 235319 (2010).

A3 P. Szumniak, S. Bednarek, B. Partoens, and F. M. Peeters, *Spin-Orbit-Mediated Manipulation of Heavy-Hole Spin Qubits in Gated Semiconductor Nanodevices*,
Phys. Rev. Lett. 109, 107201 (2012).

A4 P. Szumniak, S. Bednarek, J. Pawłowski, and B. Partoens, *All-electrical control of quantum gates for single heavy-hole spin qubits*,
Phys. Rev. B 87, 195307 (2013).

The series of papers which constitute the dissertation are preceded by an introduction and a summary of the articles (which can be treated as a guide to the articles) with a description of the novel contribution to the existing field of solid state spin based implementation of quantum computation. At the end of the thesis a summary is included.

1 Introduction, motivation and context of the thesis

In 1982, preceded by some ideas related to quantum information theory [1, 2], Richard Feynman published an original article [3] in which he suggested that the time dependent numerical simulation of a many body quantum system will be an extremely challenging task to realize using standard computers. Together with David Deutch and other researchers [3, 4, 5, 6] they proposed an alternative computer architecture - a quantum computer - which exploits the basic and counterintuitive laws of quantum mechanics (such as quantum superposition, unitary evolution and quantum entanglement) to simulate in a very efficient way quantum physical systems. Shortly after scientists discovered that such a computer can not only be used to model physical systems but also to solve other challenging computational tasks [7, 8, 9, 10, 11, 12, 13, 14]. The most profound example is the algorithm proposed by Peter Shor [9, 10] for factorization products of large prime numbers in a polynomial time while classical algorithms can solve such a problem only in an exponential time. The next important algorithm which illustrates the power of quantum computation is the Grover algorithm for searching an unsorted database [11, 12]. Scientists also realized that a physical system that will realize quantum computation is unavoidably exposed to interactions with the environment, which causes decoherence and leads to errors and the destruction of quantum information. Fortunately, Peter Shor and Andrew Steane developed methods to circumvent this problem, called quantum error correction codes [15, 16, 17, 18, 19] which allow to protect quantum information from errors of different sources (like decoherence or imperfections of the quantum gates). In the same time huge progress has been made in nanofabrication as well as in the ability to study experimentally the behavior of individual quantum objects. Furthermore, Alain Aspect in his famous experiment [20] confirmed the quantum mechanical non-local character of Nature. For all these reasons searching for physical implementations of quantum computation has attracted an enormous attention of theoreticians and experimentalists in recent years and convinced scientists that quantum computers may become reality one day. However its realization will require extreme efforts and groundbreaking ideas.

Many promising proposals for the physical realization of quantum computation have been put forward [21, 22]. The most important ones are based on semiconductor quantum dots [23, 24, 25, 26, 27], cold trapped ions [28], cavity quantum electrodynamics [29, 30, 31, 32], bulk nuclear magnetic resonance [33, 34], Josephson tunnel junctions

[35, 36, 37, 38, 39, 40], linear optics [41], molecular magnets [42, 43], spin clusters [44], single dopants in solids like donor atoms in silicon [45, 46] or nitrogen vacancy centers in diamond [47, 48, 49]. These proposals are suitable for the realization of the so called circuit model of quantum computation. There are also some other approaches like adiabatic quantum computation [50, 51, 53] or topological quantum computation [54, 55, 56, 57, 58]. The latter proposal is particularly interesting since it employs exotic quasiparticles called anyons [59, 60] (particles which obey neither fermion nor boson statistics), or Majorana bound states (particles or excitations which are in the same time its antiparticles) [61, 62] which both are due to their topological nature are much more immune to the decoherence than standard qubits from the circuit model.

From the other hand, searching for the best physical candidate for a quantum computer has stimulated enormous progress in nanofabrication and in experimental techniques which now enable measuring and controlling individual quantum objects in many different physical systems. Some of these achievements were awarded by the Nobel Prize in Physics in 2012 to the experimentalists Serge Haroche and David J. Wineland for their groundbreaking experiments on manipulating and measuring the quantum state of individual physical systems of trapped ions and photons [63, 64, 65, 66, 67, 68, 69, 70]. Furthermore, studying the behavior of individual quantum systems and especially decoherence processes, gives also a unique opportunity to investigate the fascinating physics connected with the transition from the quantum to the classical world [71, 72, 73].

Since, as suggested by Rolf Landauer, quantum computation should be realized by a “physical aparatus not Hamiltonians” [74] any physical implementation of a quantum computer architecture (within the so called circuit model) should fulfill the list of challenging and even conflicting criteria which has been put forward by David DiVincenzo [75, 23]:

i The physical system which realizes the defined basic unit of quantum information - a qubit - is needed. Usually, a qubit is encoded in a two level quantum system. Furthermore, in order to realize practical computation, scalability is required. It means that one has to be able to extend a system to a larger number of qubits arranged in a so called quantum register in which each qubit can be adressed individually (the amount of information stored in the Hilbert space should be increased exponentially without exponential cost of resources [22]).

ii Before performing computation one has to be able to initialize qubits in the quantum register in a given state with high fidelity.

iii The quantum information should be characterized by a long coherence time T_2 which is limited by the interaction with the environment. Since it is extremely difficult to isolate individual quantum systems from the surrounding environment this criterion seems to be the most challenging one. Thanks to the existence of quantum error correction codes the coherence time could be finite but has to be long enough [15, 16, 17, 18, 19], i.e. much longer than the gate operation time τ_{OP}.

iv The key criterion is the ability to control and manipulate qubits in the quantum register in a selective and precise manner to realize quantum logic gates (unitary operations) without undesired disruption of the state of other qubits in the quantum register. The one and two qubit quantum gates form a universal set of quantum gates which can realize an arbitrary quantum algorithm [76, 77]. Furthermore, as mentioned in (i) the quantum gate operation time τ_{OP} in certain proposals has to be sufficiently fast.

v When a certain quantum computation is done one has to be able to read the outcome, i.e. to make a precise measurement of the state of the qubits. It is essential that the measurement should be done on each qubit individually (selectively) without affecting the state of other qubits in the quantum register and preferably in a nondestructive manner (i.e. a projective type measurement).

There are also two additional criteria related to the quantum communication and transfer of quantum information:

vi The ability to transform stationary qubits between “flying qubits” [24, 78].

vii The possibility to transfer “flying qubits” between the desired locations.

Within this thesis we propose a set of nanodevices which are designed in such a way that they fulfill some of these demanding criteria. Our proposals belong to the spin based solid state semiconductor electrostatically defined quantum dot category [23]. First we describe the basic concepts of this original approach to quantum computation [23, 25, 26, 27] and next describe how our proposal can solve some issues related to selective single spin control. Daniel Loss and David DiVincenzo in their original work [23] proposed that a quantum bit can be encoded in the spin state of an electron (which is a natural two level quantum system) confined in an array of electrostatically defined coupled semiconductor quantum dots with electrically tunable tunnel barriers. Such electrically gated semiconductor quantum dots seem to be a very promising candidate for the realization of a quantum computer architecture since it allows to control spin qubits with electric fields, generated by top local electrodes. Two qubit gates are realized by controlling interdot coupling (switching on and off exchange interaction) by a voltage applied to the top electrodes while single electron spin qubit rotations may be realized mainly by the application of oscillating electric fields like electron spin resonance (ESR) techniques, by dragging electron wave function in inhomogeneous g-factor layer of quantum dot host in presence of static magnetic field, by optical methods, or by using the electric dipol spin resonance (EDSR) method.

Motivated by the original work [23] recently a vast number of state of the art experiments has been realized in which individual electron spins are initialized, manipulated in coherent manner and read out with high fidelity [79, 80, 81, 82, 83, 84, 85, 86, 87, 88, 89, 90, 91, 92, 93, 94, 95]. Despite these remarkable experiments, realization of a practical scalable quantum dot architecture where more than a few qubits can be manipulated selectively haven't been realized so far [1].

One of the main problems is the scalability requirement and the related difficulty in addressing individual spin qubits in a quantum register in a selective manner. The selective single electron spin control, preparation and read out seems to be more challenging than the realization of two qubit quantum gates which can be implemented by employing the electrically controllable exchange interaction in quantum dots [101] and thus realize a fully all-electrical manipulation scheme. The single spin control usually requires application of a magnetic field which causes the continuous precession of spins of all the confined qubits which prevents to address individual qubits without affecting the state of others in the quantum register. This was the motivation for a proposal in which qubits can be encoded in the singlet and triplet states of two electrons in a double quantum dot instead of using the spin up and down states of a single electron [101]. In such systems single qubit gates can be realized all-electrically but more resources are needed: two electrons instead of one for each qubit.

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[1] The proposals for other physical implementations suffer from the same limitation. The experiments are made only on a few qubits. As an example the physical implementation of Shor's algorithm has been realized, and number 15 [96, 97, 98, 99] has been factorized and recently 21 [100] which is very promising but still far from practical applications.

The first step towards the realization of selective single electron spin control was proposed in articles [102, 103, 104] where the combination of the spin-orbit interaction, the static magnetic field and the oscillating electric fields (generated by the top local electrodes) are employed in order to control the electron spin electrically - EDSR technique. Such a method was recently implemented experimentally in electrostatic quantum dots [89] and in gated nanowire quantum dots [90, 91].

Another difficulty in using electron spins confined in quantum dots as qubits is their relatively short coherence time. The main source of electron spin decoherence in semiconductor quantum dot systems at low temperatures is the hyperfine contact Fermi interaction with the nuclear spins of the host material [105, 106, 107, 108]. If no special effort is made the electron spin loses its coherence in nanoseceond timescale. Several appealing proposals have been made in order to suppress this type of decoherence to extend the electron spin coherence time from nanoseconds to microseconds and even milliseconds [109, 110]. One promising method which we consider in this thesis is to encode the qubit in the spin state of the valence hole instead of the electron [111, 112, 113]. The valence hole Bloch functions are described by p-type orbitals which vanish at the nuclear site of the host atoms and thus the contact hyperfine interaction is strongly suppressed. Unfortunately the hole spin still experiences interactions with nuclear spins which have a dipolar character which is about ten times weaker than the contact one for the electrons [114, 115, 116, 117, 118, 119, 120]. Consequently, the hole spin qubit coherence time is prolonged compared to the electron spin coherence time.[2]

These new concept proposals of electron and hole spin qubit manipulation, initialization and measurement methods have to be developed preferably all-electrical, without the need of the application of a magnetic field in any stage of the quantum computation process. In this thesis we propose several semiconductor gated nanodevices which operate on a single electron or hole spin qubit without the application of a magnetic field (except one nanodevice) which should potentially help in the realization of a scalable many qubit quantum computer. Furthermore, the proposed devices are designed in order to fulfill the criteria for physical implementation of quantum computation. This research is somehow a continuation of the pioneering work done by my promotor on the application of the electron soliton effect [121, 122, 123, 124, 125] to realize all-electrically controlled quantum

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[2] The dipolar hyperfine interaction between a hole spin state and a nucler spins for a hole occupying only heavy-hole (HH) band(i.e. absence of the heavy-hole / light-hole (LH) mixing) is of the Ising type [114, 115]. In this situation the hole spin coherence time reaches its maximum.

gates on electron spin qubits [126, 127].

The proposed devices exploit the interplay between a peculiar electron (hole) soliton effect [121, 122, 123, 124] which is present in so called induced quantum dots and wires [125] together with the spin-orbit interaction (SOI) (Dresselhaus [128] (DSOI) or Bychov-Rashba [129, 130] (RSOI) type) in order to realize various operations on single electron and hole spin states including read out, initialization and manipulation without application of a magnetic field. Since proposed devices are controlled only by weak static electric fields applied to the top local electrodes, such methods are highly suitable for addressing qubits individually and thus are promising for the realization of a scalable quantum computing architecture. In particular we propose several semiconductor gated nanodevices which are able to:

a initialize the electron spin qubit state in a given spin orientation (with [A1] or without application of a magnetic field [A2]),

b perform a read out of an electron spin (destructive [A1] or nondestructive [A2] without application of a magnetic field [A2]),

c realize motion induced rotations of HH pseudospin mediated by the DSOI, and the quantum NOT gate,

d realize an arbitrary sequence of Pauli X, Y, Z and U_S quantum gates [A4] using analogous methods as presented in the proposal from [A3] and which can be arranged in a scalable architecture [A4].

In all the proposed nanodevices a single electron or hole wave packet is confined in a semiconductor quantum well which is sandwiched between two blocking barriers. On top of this heterostructure nanostructured metal electrodes are deposited. The charge density associated with the presence of an electron or hole in the quantum well layer induces a response potential of the electron gas in the metallic gates which in turn leads to the lateral confinement of the charged particle wave function - i.e. the so called self-focusing mechanism [122]. As a result an electron or a hole is self trapped under the metal in form of a stable Gaussian wave packet which has soliton like properties. By applying a small electric field to the top metal gates one can force such a soliton to move. Its trajectory is determined by the geometry of the metal electrodes under which it moves. During the motion the electron or hole soliton maintains its shape. Furthermore, when it collides with an object - a quantum potential barrier - it can reflect or pass through it with 100%

probability and the shape of the wave packet after collision is not affected. While the electron or hole soliton behaves in “an almost” classical way, it possesses a spin which behaves fully quantum mechanically in which quantum information can be encoded.

The proposed nanodevices take also advantage of the SOI. Depending on the used material the Dresselhaus or Bychov-Rashba type of the SOI is employed. The former arises form bulk inversion asymmetry (BIA) and is characteristic for semiconductor compounds with the zinc blende crystal structure. The latter has its origin in structural inversion asymmetry (SIA) and can be induced by an electric field applied in perpendicular direction to the two dimensional electron or hole gas (which causes asymmetry in the quantum well potential profile) or structurally by using semiconductor barrier layers in a heterostructure with different band gaps to obtain asymmetric quantum well potentials. The main effect of the SOI in semiconductor nanostructures is coupling between the spin and the motional degree of freedom of an electron or hole.

In our proposals we exploit this effect in order to realize all-electrically controlled spin filtering devices and hole spin manipulation without a magnetic field. Thus the SOI can be treated as a mediator of electron or hole spin control which is realized by the electric fields.

We make a numerical time dependent simulation of all proposed nanodevices within the self consistent Poisson-Schrödinger formalism and in case of valence holes we apply additionally the four band k·p heavy-hole / light-hole model. Thus the confining potential which is felt by the electron or hole is not modeled by the approximate analytic function but determined by the solution of Poisson equation. We work within the effective mass theory which is, despite its simplicity, suitable for modeling semiconductor nanostructures of quantum dots and wires which confines single charge carriers. We apply a Poisson-Schrödinger self-consistent approach which was previously used [131] in order to model an electrostatic quantum dot which was experimentally realized [132]. The very high quantitative agreement between the theoretical and experimental results provides evidence of its correctness. Thus the presented work may be treated as a link between theoretical proposals and experimental realizations and its main goal is to stimulate experimental progress.

2 Summary of the articles which forms this thesis and conclusions

2.1 Article A1, *Nanodevice for High Precision Readout of Electron Spin*

Many extensive efforts have been made in order to develop and realize methods for an electron spin set up and read out which are two very important ingredients for the physical implementation of spin based quantum computation [75]. Most of the spin initialization techniques proposed and implemented so far in quantum dot structures exploit the application of large external magnetic field, the energy relaxation effect in the two electron quantum dot, optical methods [133, 134, 135, 136, 137], the Pauli spin blockade effect in a double quantum dot [81, 138, 139] and in nanowire quantum dots [90], while electron spin read out (single-shot read-out of an individual electron spin) utilizes mainly the spin to charge conversion method [82, 83, 86].

Within the work [A1] we propose an alternative approach and design gated semiconductor nanodevices which could serve as a single electron spin filter to accumulate single electrons in a given spin orientation in different parts of the nanodevices thus realizing an electron spin qubit initialization. Furthermore, we propose a method for electron spin read out based also on the idea of the spin filter. In both proposed devices the electron is transported within the zinc-blende semiconductor ZnTe quantum well in the $x - z$ plane sandwiched between two barriers stacked along the y axis. The considered semiconductor heterostructure is covered by metal electrodes under which the electron wave function is self focused and forms a stable soliton like wave packet [122].

Since in the considered system the electron is confined in the zinc-blende semiconductor (thus lacking crystal inversion symmetry) in the ZnTe quantum well DSOI is intrinsically present [128][3].

While in Ref. [127] DSOI was utilized to realize single electron spin rotations induced by the electron motion in an analogous manner as in the spin field effect transistor [140, 141], in the current proposal the electron trajectory can depend on its spin orientation thanks to the presence of the DSOI and this fact can be employed further to realize

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[3] We take into account only linear part of the DSOI because the quantum well height $h \approx 10$ nm is a few times smaller than the lateral diameter $d \approx 50$ nm of the induced quantum dot. The qubic Dresselhaus terms are much smaller than the linear ones to be specific they are $(\frac{h}{d})^2$ times smaller.

a spin filtering device. A similar effect of a spin dependent electron trajectory in spin-orbit coupled semiconductors was originally considered and observed within the Spin Hall Effect[4] which was predicted by M.I. Dyakonov and V.I. Perel in 1971 [143, 144] and observed very recently [145, 146].

In the first step of the filtering process the electron travels initially in the "+z" direction along the path determined by the specially designed electrodes. Due to presence of the DSOI (within the considered system) only electrons with their spin oriented either up $\uparrow$ or down $\downarrow$[5] can move straight while the electrons with other spin orientations ($\alpha \uparrow + \beta \downarrow$ where $\alpha \neq 0$,$\beta \neq 0$) turn either in the "+x" or "-x" direction and then are intercepted by the appropriate neighbor electrodes. Finally only spin up $\uparrow$ or spin down $\downarrow$ electrons can pass through this part of the nanodevice.

The main purpose of the second step of the filtering process is to spatially separate electrons with spin up orientation from those with spin down and consequently realize electron spin accumulation or read out. We present two nanodevice variants for achieving this goal. The first proposed approach is to place an diluted semimagnetic semiconductor $\mathrm{Zn}_{1-x}\mathrm{Mn}_x\mathrm{Te}$ on the electron trajectory (i.e. an area in which part of the Zn ions are replaced by Mn ions). By applying an external magnetic field in the z direction one can polarize the Mn ions. The semimagnetic area becomes a barrier or a quantum well for an electron depending on its spin orientation. Consequently, a spin up electron can pass through the semimagnetic area (quantum well) while a spin down electron is reflected from it (barrier) analogous as in the proposal presented in Ref. [147]. In this variant, the presented nanodevice can be used to realize electron spin set up or read out. The main disadvantage of this nanodevice is the necessity to apply a magnetic field in order to polarize the Mn ions. Application of an external magnetic field can lead to the persistent precession of all electron spins qubits in the quantum register and thus limits the possibility to address individual electron spin qubits.

The second designed and simulated nanodevice is an alternative proposal which does not need the application of a magnetic field to separate spin down and spin up electrons. In order to distinguish between spin up and spin down electrons after passing the first filtering part of the nanodevice, the electron reflects from a potential barrier which is formed under a 45° cut corner edge of the electrode and starts to move in the "+x"

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[4] This term was introduced in 1999 by J. E. Hirsch [142].

[5] The electron spin orientation is defined as an expectation value of the spin operators $\vec{s} = \langle \frac{\hbar}{2}\vec{\sigma} \rangle$ where the $\vec{\sigma}$ is the vector of the Pauli spin matrices. We use a convention where the spin up (down) orientation corresponds to the $s_z = \frac{\hbar}{2}$ ($s_z = -\frac{\hbar}{2}$).

direction. Then due to the presence of the DSOI, electrons with initial spin up (down) state are directed to the channel in the upper (lower) part of the nanodevice. Thus by measuring the presence of the electron either in the lower or upper channel (i.e. by utilizing a quantum point contact (QPC) [148]) one can identify what was the initial value of the electron spin. In this proposal, at the moment of the measurement, the electron spin is no longer in the same state as it was initially, because after reflection in the "+x" direction the electron motion started to induce electron spin rotation around the axis parallel to the direction of the electron motion. The measurement of an electron spin in this proposal has thus a destructive character. Since the electron's trajectory strongly depends on its initial spin the proposed read out scheme is very precise. The proposed nanodevices can naturally be integrated with the nanodevices capable to realize basic quantum gates on single electron spin qubits as presented in Ref. [127].

2.2 Article A2, *Spin accumulation and spin read out without magnetic field*

A continuation of the research on the design of nanodevices for electron spin qubit read out and set up [A1] is presented in article [A2]. As mentioned in the introduction, all-electrical magnetic free control of electron or hole spins seems to be a very appealing method to address individual qubits in a quantum register without disturbing the state of other qubits, which is essential for realizing a scalable quantum computer architecture. In the original article [126], such an all-electrical control of the electron spin was proposed and appropriate nanodevices were designed and simulated. If one wants to apply such nanodevices for quantum computation purposes, the electron spin initialization as well as the read out have also to be realized without application of a magnetic field. In the article [A2] we propose such devices which are new and improved in comparison to nanodevices from the previous proposal [A1]. They can be naturally integrated with devices from Ref. [126]. One of the currently proposed devices [A2] is capable of the realization of a magnetic free electron spin accumulation for electron spin qubit initialization purposes. The second one is suitable for a nondestructive read out of the electron spin in the sense that it can answer the following question ”is the electron in the spin up state?”. The proposed method is unique since, as far as we know, there are no experiments and even theoretical proposals where the single electron spin can be initialized or read out completely without application of a magnetic field in semiconductor quantum dot systems. Which is also very important and desired is the fact that the read out is realized in a nondestructive manner (i.e. a projective type measurement). Furthermore, electron spin initialization and read out is realized in an ultrafast manner (sub nanosecond) and with very high fidelity reaching 99%.

In order to avoid interaction with non zero nuclear spins of the host material which leads to an electron spin dephasing [6] [105, 106, 107, 108] we replace ZnTe by Si which can be prepared in a form with more than 99% from nuclear spin free isotopes (i.e. ^{28}Si). Therefore, the coherence time of the electron spin qubit confined in a Si quantum well is significantly prolonged.

Since we are dealing now with Si as host material (with a cubic diamond crystal structure) Dresselhaus coupling is no longer present in the system. In the current proposal [A2] we employ instead the RSOI. The RSOI interaction couples the spin and charge degree of freedom of an electron in such a way that when the electron moves, its spin is rotated around the axis perpendicular to the direction of motion. Furthermore, in presence of RSOI spin dependent transport can also be realized and the straight motion of an electron along x axis is only possible if its spins is oriented up or down. Such a motion does not affect the electron spin. We use the system of coordinates where the quantum well is placed in the y direction.

The spin preparation process as well as the spin read out realized by the proposed nanodevices is divided into two main steps. In both proposed devices the first step of the accumulation as well as read out process is almost identical as in the previous proposal [A1], but because this time the Rashba SOI is employed, electrons are moving initially along the path in the "+x" direction (not in "+z") and electrons whose spin was not oriented exactly in "+z" or "-z" direction due to the presence of RSOI are altered either in plus or minus z direction. Thus this part of the nanodevice plays the role of the spin filter where only electrons with spin up or down can be selected and pass through.

In the next step of the spin set up and spin read out process, the spin up and spin down electrons are distinguished and are directed to different parts of the nanodevice. In order to realize electron spin accumulation we use a nanodevice where the electrodes which cover the nanodevice are designed in such a way that after passing the first filtering part the electron reflects from the cut corner electrode, turns by 90° and then starts to move in the "+z" direction. Just after reflection its momentum vector points exactly in the "+z" direction. Then, due to the presence of RSOI, the trajectory of a spin up electron

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[6] As a consequence if no special effort is made the electron spin loses its coherence in a ns timescale

is curved to the right (“+x”) while a spin down electron is directed to the left (“-x”). After the reflection, the electron motion starts to induce electron spin rotation. Fortunately, after traveling a distance λ_{SO} the electron spin is restored (a full 2π angle rotation is realized) and the electron trajectory becomes parallel to the “z” axis again while the spin up and spin down electrons are now separated spatially. Then the electron is reflected from the 45° cut corner edge of the electrode. (Thanks to the fact that just before the reflection the electron momentum $\vec{p}$ points exactly in the “+z” direction, it is possible to obtain a smooth 90° reflection.) The electron with spin down orientation reflects in the “-x” direction while a spin up electron is reflected in the “+x” direction. Then both move straight. Since now the electron spin is oriented either up or down it does not precess during its motion (precession around the “z” axis). Thus at the end, an electron with spin up will accumulate in one part of the nanodevice and move in the “+x” direction while an electron with spin down will move in the opposite “-x” direction in another region of the proposed nanostructure. Electrons with such a prepared spin state can be transported to nanodevices that act as quantum gates on single electron spin states [126].

The second nanodevice is capable to measure the spin state of the electron without affecting its spin state after the read out process. The measurement is performed in such a way that the answer to the following question is provided ”is the initial electron spin oriented up?” The measurement is based on the idea of checking the presence of the electron under “a control quantum dot”. The nanodevice acts as follows. After the first step of the filtering process, the electron is reflected. Depending on its spin orientation it will follow two different trajectories. If the electron spin was initially oriented up it travels along a certain path (omitting the region with “the control quantum dot”) and then returns to its initial position. Consequently, there is an absence of the electron in the controlling quantum dot. Thus by measuring the presence or the absence of the electron in the region of the control quantum dot (i.e. by the QPC method) one can indicate what was the initial value of the electron spin. The presence of the electron means that initially the electron spin was oriented down and the answer to the asked question is negative and the electron spin state is destroyed. Such a method does not require application of an external magnetic field. Proposed devices can be naturally integrated with the quantum gates proposed in a recent article [126]. Moreover, the proposed nanodevices are also suitable for acting on the spin state of a single valence hole confined in zinc blende semiconductors in which the DSOI is present. The difference will be in nanodevice size which is determined by the λ_{SO}, and the electrodes’ arrangement which have be rotated by the 90° with respect to the current orientation.

2.3 Article A3, *Spin-Orbit-Mediated Manipulation of Heavy-Hole Spin Qubits in Gated Semiconductor Nanodevices*

Many experiments [112, 149, 150, 151] have shown that the interaction between a hole spin and nuclear spins of the host material is significantly weaker than for the electron spin, thus making a spin of a valence hole confined in semiconductor nanostructures an attractive candidate for a robust solid state spin qubit, and a promising alternative for the electron spin qubit. However, there are only few theoretical proposals on how to control HH spin qubits [152, 153, 154, 155, 156]. Several experiments exist based mainly on optical methods, in which the hole spin states in quantum dots [157, 158, 159, 160, 161, 162, 163, 164] are controlled. Most of them require the application of a magnetic field. Very recently, all-electric hole spin manipulation in gated semiconductor nanowires has also been demonstrated [165]. Within the work [A3] we present a new and promising method for controlling HH spin qubits in semiconductor nanostructures without application of a magnetic field. In particular we show that the motion of a hole along an induced quantum wire [125] in presence of DSOI can induce coherent rotations of the HH spin (more precisely of the pseudo spin 1/2) state. We further exploit this observation to realize an all electrical-control scheme for the HH spin qubit. The motion of the hole along a certain direction is equivalent to the application of an effective magnetic field which cause the heavy-hole spin to rotate in a coherent manner. This method seems to be more suitable for the coherent manipulation of a HH spin than the application of a real magnetic field which, due to the small hole in plane g factor, has to be very high (several Teslas) in order to rotate the hole spin. The application of such a high external magnetic field is possible but still very challenging in experiments. The proposed all-electrical HH spin control circumvents this problem. We make calculations within the k·p HH-LH multiband model and show that in the investigated systems the hole occupies mostly the HH band which is caused due to the strong confinement in the quantum well growth direction. This is an important result which allows to encode the qubit in HH spin basis states. As suggested, only in systems with negligible HH/LH band mixing the coherence of a hole spin state is significantly (about ten times) prolonged compared to the electron spin coherence time [114, 115, 116, 117, 118, 119, 120]. By analyzing HH spin rotations in the investigated system, we numerically estimate the λ_{SO}[7] parameter for different materials: GaAs, CdTe, ZnTe. Moreover the form of rotation operators which act on a HH spin while the hole is moving are provided.

Based on these results we put forward a proposal of a GaAs nanodevice which can realize a quantum NOT gate on a HH spin qubit. In order to realize this operation, the hole is transported around a closed rectangular loop which is determined by the geometry of specially designed top metal electrodes. During the realization of the proposed gate, the hole passes each segment of the loop and an appropriate set of π and $\pi/2$ rotations is made. Finally, the quantum NOT logic operation is performed. Since the hole is transported to the initial position, the required quantum operation is performed exclusively on its spin state. The quantum NOT logic operation is realized within sub nanoseconds ($\tau_{OP}^{GaAs} \sim 250$ picoseconds). If the hole spin coherence time reaches $T_2 = 100$ picoseconds, as suggested by the experiment [112] it is potentially possible to reach the threshold for application of quantum error correction codes (defined by the ratio of coherence time and gate operation $\frac{\tau_{coh}}{\tau_{op}}$), which typically varies between 10^{-5} and 10^{-3} [15, 16, 17, 18, 19].

2.4 Article A4, *All-electrical control of quantum gates for single heavy-hole spin qubits*

The all-electrical concept of manipulating the spin states of a hole via controlling its motion introduced in previous article [A3] is extended in the current proposal [A4].

The design of a set of nanodevices which can realize basic quantum logic gates on a single HH spin qubit is put forward [A4]. In particular, we propose nanodevices which can realize Pauli X, Y and Z gates suitable for the realization of π angle rotations of a HH spin qubit around the x, y, and z axis, respectively. We also design a nanodevice which can realize an operation which we call the U_S gate: $\pi/2$ angle rotation of the HH spin and at the same time the operation is capable to create (or destroy) a balanced superposition of the basis states of the qubit. Moreover we design a nanodevice covered by a system of metal gates which can realize an arbitrary sequence of all previously proposed quantum logic gates. Each quantum gate is realized by transporting the hole along a special trajectory - a closed rectangular loop - determined by the shape of the surface electrodes. During the motion along the loop a certain sequence of π and $\pi/2$ HH spin rotations are performed, which results in the realization of the desired quantum gate. Motion of the hole along

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[7] Distance which has to be traveled by the hole in order to realize full 2π HH spin rotation.

certain directions induces HH spin rotations and special operators can be associated with this process which were introduced in [A3]. The topology of the metal gates is deduced from the form of these operators.

Since the proposed all-ellectric HH spin control method allows for addressing individual qubits we also show how such a device can be arranged in a quantum register to form a scalable architecture for quantum computation applications.

The presented nanodevices in [A4] are now based on CdTe, while the proposals in [A3] were based on GaAs. This allows to obtain smaller and faster devices as well as potentially longer coherence times of the hole spin confined in it. Furthermore, the proposed gates are characterized by a very high fidelity reaching 99%.

Summary

In this thesis we design, model and present results of time dependent simulations of semiconductor nanodevices which can be utilized as basic building blocks of a future quantum computer. In the designed nanodevices, the basic unit of quantum information - a qubit - is encoded in the spin (intrinsic angular momentum) of a single electron or hole confined in the semiconductor nanostructure in which induced quantum dots and wires are formed.

The proposed nanodevices are designed in such a way that they fulfill the basic criteria of physical implementation of quantum computation: the ability to initialize and read out (possibly in nondestructive or projective type manner) the state of a qubit respectively before and after realization of a certain quantum algorithm, the capability to realize fully controllable manipulation on a qubit, i.e. the realization of one and two qubit quantum logic gates. Furthermore, the qubit should be characterized by a long coherence time. The whole quantum computer architecture should fulfill the scalability requirement which means that it should be possible to build quantum registers composed of many qubits, which one can control individually without disturbing the state of other qubits in the register.

In particular we have designed and simulated nandevices which are capable to initialize and read out the spin state of the electron, and devices which are able to manipulate the spin state of a single hole by the application of single quantum logic gates. We have also designed a so called ”combo” nanodevice in which arbitrary sequence of proposed single quatum logic gates can be realized as well as a fragment of a scalable architecture

composed from such ”combo” nanodevices, containing four hole spin qubits.

The fact that spin manipulation, initialization and read out realized by the proposed nanodevices does not require the application of a magnetic field (except one nanodevice form Chapter 3) makes our proposals particularly interesting and unique among other proposals based on electron and hole spin qubits in semiconductor nanostructures. The proposed devices operate on spin qubits using exclusively weak static electric fields, which are locally generated by the voltages applied to the metal electrodes deposited on top of the investigated nanostructure. It allows to control individual qubits in the quantum register without disturbing the state of other qubits, which is very important for the realization of a scalable architecture.

Control of electron (hole) spin qubits without a magnetic field is possible thanks to the interplay between the spin-orbit interaction and the self-focusing effect of an electron (hole) wave function which is present in induced quantum dots and wires. The former effect couples the motional and spin degree of freedom of an electron (hole) enabling motion induced spin rotation of a single charge carrier or vice versa, resulting in a spin dependent particle trajectory. While the latter effect allows for transport of an electron (hole) in the form of a stable soliton-like wave packet which motion is controlled by the voltage applied to the metal gates as well as the gate geometry which determines the particle path. Spin rotations induced by the particle motion are employed in order to realize single spin qubit quantum gates, while the effect of the spin dependent trajectory is used to realize spin filtering devices which aim is to initialize and read out the spin state of a single charge carrier.

In order to prolong the electron spin qubit coherence time which is limited by the contact hyperfine interaction with nuclear spins, Si nuclear free material can be applied in the proposed nanodevices. Alternatively, the qubit can be encoded in the more immune to the decoherence spin state of a hole.

Furthermore, the proposed devices also make possible a fully controllable transport of electrons or holes, which spins carry the quantum information, and thus may be also useful for transferring the quantum information within the semiconductor nanostructures. Consequently, they may find applications for quantum communication in semiconductor nanostructures.

We have performed numerical (time dependent) simulations of all of the proposed nanodevices by solving iteratively the time dependent Schrödinger equation (within the effective mass theory) together with solving the Poisson equation in each time step of the numerical procedure in the three dimensional computational box containing the entire nanodevice. Similar methods were previously employed by my promotor in order to model (reproduce) theoretically with very high accuracy reach set of experimental results about properties of electrostatic quantum dots. Thus our work can be considered as a link between the theoretical proposal and an experimental realization.

Thanks to the fact that the proposed nanodevices realize operations within sub-nanoseconds on a spin qubit which is characterized by a coherence time of the order of hundreds of nanoseconds, their experimental realization would be an important step towards the physical implementation of quantum computers.

Podsumowanie

Niniejsza praca dotyczy projektowania, modelowania i komputerowej symulacji działania półprzewodnikowych nanourządzeń, które mogą być wykorzystane jako podstawowe elementy przyszłego komputera kwantowego. W projektowanych nanourządzeniach nośnik informacji kwantowej - kubit jest realizowany przez spin (wewnętrzny moment pędu) pojedynczego elektronu lub dziury uwięzionych w nanostrukturze półprzewodnikowej. Urządzenia zaprojektowane są w taki sposób aby spełniały podstawowe kryteria fizycznej implementacji komputerów kwantowych. Wymagają one między innymi możliwości precyzyjnego ustawiania stanu kubitu na początku realizowanego algorytmu kwantowego i odczytu (najlepiej w sposób nieniszczący lub rzutowy) na jego końcu oraz wykonywania w pełni kontrolowanych operacji na kubicie - realizacji jedno i dwukubitowych kwantowych bramek logicznych. Cała architektura komputera kwantowego musi ponadto spełniać kryterium skalowalności tzn. układ powinien się dać rozszerzyć na większa liczbę kubitów (rejestr kwantowy), które można w indywidualny sposób kontrolować nie zaburzając stanu pozostałych kubitów w rejestrze.

W pracy zaprojektowano nanourządzenia służące do ustawiania i odczytu spinu pojedynczego elektronu, oraz do wykonywania operacji jednokubitowych bramek kwantowych na spinie pojedynczej dziury. Zaproponowano również nanourzadznie “combo”, w którym może być wykonana dowolna sekwencja jednokubitowych bramek kwantowych oraz zaprojektowano fragment skalowalnej architektury składającej się z takich nanourządzeń.

Niezwykle istotną cechą, odróżniającą nasze rozwiązania od innych dotychczasowych propozycji realizacji obliczeń kwantowych w nanostrukturach półprzewodnikowych jest możliwość ustawienia i odczytu spinu pojedynczego nośnika ładunku oraz wykonania na nim innych operacji bez użycia zewnętrznego pola magnetycznego (z wyjątkiem jednego nanourządzenia z rozdziału (3)). Operacje wykonywane przez zaprojektowane nanourządzenia kontrolowane są wyłącznie przy użyciu słabych statycznych pól elektrycznych, które są generowane lokalnie przez napięcia przyłożone do metalowych elektrod ułożonych na powierzchni nanostruktury. Dzięki temu możliwa jest kontrola pojedynczych kubitów w rejestrze kwantowym bez zaburzania stanu pozostałych kubitów, co jest warunkiem realizacji skalowalnej struktury.

Kontrola spinu elektronu (dziury) bez użycia pola magnetycznego jest możliwa dzięki wykorzystaniu oddziaływania spin-orbita oraz efektu samoogniskowania funkcji falowej elektronu (dziury) wywołanego oddziaływaniem nośnika ładunku z ładunkiem indukowanym na metalowych elektrodach ułożonych na powierzchni nanostruktury. Pierwszy efekt wiąże ruch elektronu (dziury) z ich stanem spinowym co umożliwia realizację obrotu spinu powodowanego przez ruch nośnika ładunku lub odwrotnie uzyskanie trajektorii cząstki zależnej od jej stanu spinowego. Natomiast drugi efekt pozwala na kontrolowany napięciami przyłożonymi do metalowych elektrod transport elektronu (dziury) w postaci stabilnego pakietu falowego mającego charakter solitonu. Obroty spinu indukowane ruchem wykorzystane są do realizacji jednobitowych bramek kwantowych, natomiast efekt zależnej od spinu trajektorii do realizacji filtrów spinowych mających za zadanie ustawiać i odczytywać stan spinowy pojedynczego nośnika ładunku. Ze względu na fakt, że zaprojektowane nanourządzenia umożliwiają kontrolowany transport elektronów lub dziur, których spin jest nośnikiem informacji, mogą być przydatne do przesyłania informacji kwantowej wewnątrz półprzewodnikowych nanostruktur i tym samym znaleźć zastosowanie w komunikacji kwantowej w nanoukładach półprzewodnikowych.

Ponieważ algorytmy wykonywane przez komputer kwantowy będą obejmowały conajmniej kilka tysięcy operacji, które łącznie muszą być zrealizowane w czasie mniejszym od tzw. czasu koherencji, kubit powinien być realizowany przez stan kwantowy który zachowuje koherencję odpowiednio długo. Zakodowanie informacji kwantowej w stanie spinowym dziury pozwala wydłużyć czas koherencji w porównaniu z kubitem zrealizowanym na stanie spinowym elektronu. Ponieważ proponowane nanourządzenia wykonują operacje w czasie rzędu ułamków pikosekund na kubicie, którego czas koherencji jest rzędu setek nanosekund, ich eksperymentalna implementacja może być ważnym krokiem w kierunku fizycznej realizacji komputerów kwantowych.

W pracy wykonano numeryczne symulacje działania wszystkich zaproponowanych nanourządzeń poprzez iteracyjne rozwiązywanie zależnego od czasu równania Schroedingera z jednoczesnym obliczaniem aktualnego potencjału uwięzienia i pola elektrycznego poprzez rozwiązywanie w każdej chwili czasowej równania Poissona w trójwymiarowym obszarze przestrzennym obejmującym nanourządzenie. Identyczne metody obliczeniowe pozwoliły w przeszłości odtworzyć bogate spektrum wyników eksperymentalnych dotyczące własności elektrostatycznych kropek kwantowych. Dzięki temu niniejszą pracę można traktować jako ogniwo łączące teoretyczny opis nanourządzenia z jego eksperymentalną realizacją.

Samenvatting

In deze thesis ontwerpen, modelleren en simuleren we halfgeleider nanodevices die gebruikt kunnen worden als bouwstenen van een toekomstige kwantumcomputer. In deze nieuw ontworpen nanodevices wordt de basiseenheid van kwantuminformatie - de qubit - gecodeerd in de spin van een elektron of holte, opgesloten in de halfgeleider nanostructuur waarin kwantumstippen en draden gemaakt zijn.

De voorgestelde nanodevices zijn zodanig ontworpen dat ze voldoen aan de basis criteria voor de fysische implementatie van kwantumcomputatie. Deze basis criteria zijn de mogelijkheid om de toestand van een qubit te initialiseren en uit te lezen na de uitvoering van een zeker algoritme (en mogelijk in een niet-destructieve manier), en de volledig controleerbare manpulatie van deze qubit, i.e. de realisatie van een of twee-qubit logische operaties. Daarnaast moet de qubit gekarakteriseerd worden door een lange coherentietijd. De gehele computerarchitectuur moet ook volledig schaalbaar zijn, wat betekent dat het moet mogelijk zijn om kwantumregisters op te bouwen uit vele qubits, die individueel gecontroleerd moeten kunnen worden zonder de toestand van andere qubits in het register te verstoren.

In het bijzonder hebben we nanodevices ontworpen en gesimuleerd die het toelaten om de spin van een elektron te initialiseren en uit te lezen, en devices waarin de spin van een holte kan gemanipuleerd worden door kwantum gates. We hebben ook een ”combo” nanodevice ontworpen waarin een arbitraire opeenvolging van kwantum logische gates kan gerealiseerd worden. En eveneens hebben we een onderdeel van een schaalbare architectuur opgebouwd uit dergelijke ”combo” devices, met vier holte spin qubits.

Het feit dat spin manipulatie, initialisatie en uitlezing in de voorgestelde nanodevices geen gebruik maken van een uitwendig aangelegd magneetveld (behalve één nanodevice in hoofdstuk 3) maakt onze voorstellen uniek onder de voorstellen gebaseerd op elektron en holte qubits in halfgeleider nanostructuren. De voorgestelde devices manipuleren de spin qubits enkel met statische elektrische velden die lokaal gegenereerd worden door spanningen aan te leggen op metaal elektrodes bovenop de nanostructuren. Het laat toe om individuele qubits te manipuleren in het kwantumregister zonder de toestand van andere qubits te verstoren, essentieel voor de realisatie van een schaalbare architectuur.

Controle over de elektron (holte) spin qubits zonder een magneetvled is mogelijk door de combinatie van de spin-baan interactie en het zelf-focusing effect van een elektron (holte) golffunctie die aanwezig is in ge?nduceerde kwantumstippen en draden. Het eerste effect koppelt de bewegings vrijheidsgraad met de spin vrijheidsgraad van een elektron(holte) wat leidt tot spin rotatie ge?nduceerd door de beweging van het deeltje en vice versa. Dit resulteert in een baan die afhankelijk is van de spin. Het tweede effect leidt tot het transport van een elektron (holte) in de vorm van een soliton-achtig golfpakket waarvan de beweging bepaald wordt door de spanning aangelegd op de metaal elektroden en door de geometrie van deze elektroden. Spin rotaties die door de beweging ge?nduceerd worden worden gebruikt om één spin kwantum gates te realizeren, terwijl het spin afhankelijke traject gebruikt wordt om een spin filter te realizeren. Een spin filter wordt dan weer gebruikt voor de initialisatie en uitlezing van de spin toestand van een enkele spin ladingsdrager.

Om de elektron spin coherentietijd, die gelimiteerd wordt door de hyperfijn interactie met de nucleaire spins, te verlengen kunnen we de voorgestelde nanodevices realiseren in Si. Een alternatief is om de qubit te coderen in de spin toestand van een holte die meer immuun is voor decoherentie.

Daarnaast maken de voorgestelde devices ook het controleerbaar transport mogelijk van elektronen of holten waarvan de spin de kwantum informatie dragen, en kunnen dus ook nuttig zijn voor de transfer van kwantuminformatie in halfgeleider nanostructuren.

We hebben in deze thesis numerieke (tijdsafhankelijke) simulaties uitgevoerd van alle voorgestelde nanodevices door iteratief de tijdsafhankelijke Schrödingervergelijking op te lossen (binnen de effectieve massa benadering) samen met de Poisson vergelijking, in elke tijdsstap van de numerieke procedure in een drie-dimensionale doos die het hele nanodevice bevat. Analoge methoden werden reeds gebruikt door mijn promoter om theoretisch een aantal resultaten i.v.m. de eigenschappen van elektrostatische kwantumstippen erg accuraat te modelleren. Daarom kan deze thesis beschouwd worden als de link tussen een theoretisch voorstel en de experimentele realisatie.

Dankzij het feit dat de operaties in de voorgestelde nanodevices gerealiseerd worden in subnanoseconden op een spin qubit die gekarakteriseerd wordt door een coherentietijd van de orde van honderden nanoseconden, kan hun experimentele realisatie een belangrijke stap zijn in de fysische implementatie van een kwantumcomputer.

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