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Quantum transport phenomena of two-dimensional mesoscopic structures

PhD Theses

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1 Introduction

Mesoscopic systems are of special interest, since they are situated between macro- and microscopic worlds, the former of which is non-quantum physical, whereas – to our present knowledge – the latter should be described according to the rules of quantum physics. The mean free path of electrons at low temperatures ($\sim$ mK) is typically $100 - 1000\,\mathrm{nm}$. The phase coherence length, which describes the distance along which the electron, as a wave, maintains its ability to interfere with itself in spite of being scattered in the sample, has in general the same order of magnitude as the mean free path. When the spatial extension of the investigated system is comparable to the mean free path of carriers, quantum mechanical interference effects cannot be omitted.

In semiconductor heterostructures, the confinement perpendicular to the interface of the different materials results in the formation of so-called two-dimensional electron gas (2-DEG) close to the contact layer. The coherence length of the conductance band electrons can be extremely high in these systems. Considering the example of GaAs/AlGaAs systems, one of the reasons for this effects (and the high mobility of the electrons) is the spatial separation between the donor atoms in the AlGaAs layer and the conduction electrons in the GaAs layer. As a consequence, quantum mechanical interference phenomena play a crucial role in the conductance properties of these heterostructures.

Besides fundamental aspects, an additional important reason for investigating these systems is the possibility of applications, which originates from the experimental control of spin-dependent properties. Spin splitting in the 2-DEG results from two distinct effects. Our work focuses on the so-called Rashba-type spin-orbit interaction (SOI) [1]. In contrast to the Dresselhaus effect [2], Rashba-type SOI is not related to bulk properties. As it has been demonstrated [3], this kind of interaction is present only in semiconductor heterostructures with a lack of inversion symmetry in the growth direction. The experimental control of the strength of the Rashba-type SOI stems from the fact that the confinement-related structure inversion asymmetry can be tuned by external gate voltages. Several experiments have already demonstrated that the Rashba parameter α can be modified in this way [4, 5], leading to a strong modulation of transport and spin dependent properties of the related devices.

Active manipulation of the spin degree of freedom mainly for information processing purposes is the subject of spintronics, which is related to a large class of spin transformation effects and possible applications. One of the first proposals in this field was the Datta-Das spin field-effect transistor (SFET) [6] the purpose of which is the control of the spin current with a gate voltage. Spin transport differs from charge transport in that spin is not a conserved quantity due to spin-orbit interactions mentioned above and the hyperfine coupling. Studies in the field of spintronics include investigations of spin transport in electronic materials as well as quantum computation with spin-based qubits [7]. Within a wider context, the fundamental goal of spintronics is to understand the interaction between the particle spin and its solid-state environment – in order to use this knowledge to create functional devices [8].

2 Motivation and goals

Nowadays the physics of mesoscopic objects and quantum theory of various spin systems are in the focus of numerous experimental and theoretical studies. The main reason for this is twofold: the appearance of fundamental interference phenomena in solid state systems and its possible applications. Let us recall that state of the art experimental techniques allow the fabrication of samples that are interesting from both aspects. E.g., GaAs-AlAs periodic structures can be prepared by molecular-beam epitaxy (MBE) [9], and InAlAs/InGaAs based heterostructures [10] or HgTe/HgCdTe quantum wells [11] are also relevant from our point of view.

The main goal of our investigation was to determine the conductance properties of nanoscale superlattices in the presence of Rashba-type SOI. The electronic transport strongly depends on the experimentally controllable SOI strength. According to our concept, the building elements of these lateral networks are simple straight nanowires, the combination of which can create closed paths for the electrons. We were motivated by the possibility of preparing spin-polarized (pure) states at the output of the device, which is of outstanding importance for spintronic applications. Multiple quantum mechanical interference in the closed loops can lead to this polarization effect.

More generally, the aim of many scientific projects is to reveal new concepts underlying spintronic applications (for instance, quantum logic gates). In my opinion, one of the most important and exciting scientific questions of the 21st century is in which way we can realize quantum data processing and computing. Nowadays, the rapid development of nanosciences led to the discovery of new materials (called nanomaterials) and novel fabricating techniques for them. Additionally, theoretical models and methods have also been developed in the course of years, which means a promising combination for the realization of information processing on quantum mechanical grounds.

3 Investigated topics

1. We considered nanoscale systems in which the electrons taking part in spin and charge transport can propagate in single mode narrow quantum channels which are the building blocks of two-dimensional infinite superlattices or finite nanostructures. The transport properties of these systems are determined by i) interference of the high mobility electrons, ii) the strength of the Rashba-type spin-orbit interaction, and iii) the geometry of the superlattice. Our main goal to obtain a spin-dependent band scheme of infinite lattices, i.e., the determination of the dispersion relation $E_{n,m}(\mathbf{k})$, where the band indices n and m are related to the spatial periodicity of the artificial electron crystal.

2. According to the Landauer-Büttiker formalism [12], the conductance G of a quantum wire is proportional to the transmission probability T of electrons which can move along the waveguide:

$$G(E) = \frac{2e^2}{h} MT(E), \tag{1}$$

where the number of conducting modes is denoted by M. (In our work we always assume $M = 1$.) We investigated the conductance properties of relatively large, but finite lattices. The transmission probabilities for electrons with different spin orientation depend on the strength of the spin-orbit interaction. The conductance also shows spin-dependent behaviour, offering various possible spintronic applications. We determined the conductance properties of finite arrays at high temperatures as well.

3. We have also considered time-dependent transport phenomena in simple polygon geometries. The dynamics of the electrons propagating in narrow quantum channels is influenced by an oscillating Rashba-type SOI. That is, the Hamiltonian we consider depends on time via the spin-orbit coupling term.

4 Applied models and methods

Our models are superlattices and loop geometries which represent nano-scaled devices that are connected to input and output arms. They consist of narrow quantum wires in which the charge carriers can propagate in the presence of Rashba-type spin-orbit coupling.

The Hamiltonian with a Rashba-type spin-orbit interaction term, which can describe the behaviour of electrons in the $x - y$ plane, is given by

$$H = \hbar\Omega \left[\left(-i\frac{\partial}{\partial s} + \frac{\omega}{2\Omega}\mathbf{n}(\sigma \times \mathbf{e}_z) \right)^2 - \frac{\omega^2}{4\Omega^2} \right], \tag{2}$$

where the unit vector $\mathbf{n}$ points to the chosen positive direction along the wire and we defined the characteristic kinetic energy $\hbar\Omega = \hbar^2/2m^*a^2$ (with a being one of the lattice constants). The strength of the SOI is given by $\omega/\Omega = \alpha/a\Omega$, where the Rashba parameter α is a function of the electric field applied in the z direction [13], and s denotes the dimensionless length variable along the channel measured in units of a.

In order to find an eigenstate for the whole geometry, we apply appropriate boundary conditions [14]: the solutions have to be continuous at the junctions, and we also require the net spin current density to be zero at these points.

For an infinite periodic structure, the Bloch-wave solutions have the following form

$$\Psi(\mathbf{r}) = \varphi(\mathbf{r}) e^{i\mathbf{kr}}, \tag{3}$$

with lattice-periodic spinors $\varphi(\mathbf{r})$ and two-dimensional wave vectors $\mathbf{k} = (k_1, k_2)$. It means an additional, special boundary condition that follows from the Bloch theorem [15]. The consequence is an energy spectrum with a specific structure: e.g., there will be no solutions in certain energy ranges. Determination of the band structure means finding triplets $\{E(\mathbf{k}), k_1, k_2\}$ that correspond to a Bloch-wave eigenspinor of the problem.

In case of a finite structure (with a size of $N \times N$, where the N is an integer denoting the number of the junctions), the Landauer formula (Eqs. 1) provides the conductance. $G(E)$ depends on the SOI strength via the transmission probabilities.

At finite temperatures, the electrons which are relevant in transport processes, are not modelled by monoenergetic states. Additionally, in a large, or even mesoscopic system, transport will not be ballistic and quantum mechanical coherence of the carrier wave functions will not be maintained over the whole device. In order to take this issue into account, we introduce random, independent point-like scattering centers in the network. The considered interference phenomena in the network are spin sensitive, thus the scatterers are taken to be spin-dependent.

Quantum systems often interact with time-dependent external fields (for instance, they can be driven by a laser pulse). In our case the time-dependence enters via the strength of the Rashba-type SOI term. This means that the Hamiltonian (Eqs. 2) is modified: the constant value of ω is replaced by $\omega(t) = \omega_0 + \omega_1 \cos(\nu t)$, where ν denotes the driving frequency. Then the problem is equivalent to the solution of the time-dependent Schrödinger equation with a Hamiltonian being periodic in time. To this end we applied Floquet's theory [16] to obtain the quasi-energies and quasi-eigenstates, and observed the appearance of high harmonics ($n\nu$) in the time evolution.

5 New scientific results

1. We calculated the eigenspinors and eigenenergies of the Hamiltonian describing the motion of an electron in a one-dimensional quantum wire under the influence of static Rashba-type SOI. We determined the spin-dependent subband (miniband) structure of an infinite superlattice structure whose building blocks are narrow, single mode quantum wires. The position and width of the subbands were found to be determined by the geometric parameters of these artificial crystals and the strength of the Rashba-type SOI [III.].

2. We determined the conductance properties of networks that can be considered as finite parts of the infinite superlattices discussed in the previous point. It was found that the subband structure determines the energy dependence of the low temperature conductance already for relatively small networks (containing 5×5 junctions or more). Specifically, according to our calculations, the conductance of the finite networks is practically zero at energies that correspond to the mini-bandgaps of the infinite superlattice [III.].

3. The conductance of the finite arrays has also been determined at finite temperatures. We found that unless no other conducting modes than the transversal ground state is excited, the high temperature conductance is independent of the value of the Fermi energy. Additionally, we found that the conductance of the device can be controlled using the experimentally adjustable spin-orbit interaction strength even in the high temperature range. According to our analysis, the physical background of this result is the dependence of the subband structure on the SOI strength: there are no mini-bandgaps for zero SOI, but they appear and get wider as the SOI becomes more pronounced [II.].

4. It has been investigated how dephasing effects modify the conductance properties of finite networks. To this end, we introduced random, independent Dirac δ scatterers that are situated at the junctions. We observed that although the details of the conductance as a function of the Fermi energy and the strength of the spin-orbit interaction are smeared out, the miniband related qualitative picture remains valid even when the conductance is strongly suppressed due to scattering events. Consequently, it is possible to control the conductance of the network via the tuning of the strength of the SOI also in the presence of dephasing effects [II.].

5. We demonstrated the emergence of propagating electron density and spin polarization waves in two-terminal nanodevices in which the time-dependent oscillating SOI is present. These simple loop geometries can be used as sources of spin-polarized wavepackets even for a completely unpolarized input. According to our calculation, this dynamical spin polarization effect appears for realistic, experimentally achievable parameter ranges and remains also observable when moderate intensive scattering processes are taken into account. Our model suggests a novel source of spin-polarized electrons that can be realized with pure semiconducting materials without the use of external magnetic fields [I.].

Publications

Publications discussed in the dissertation:

[I.] **V. Szaszkó-Bogár**, P. Földi, F. M. Peeters,

Oscillating spin-orbit interaction as a source of spin-polarized wavepackets in two-terminal nanoscale devices,

J. Phys.: Cond. Matt. **26**, 135302 (2014).

[II.] P. Földi, **V. Szaszkó-Bogár**, F. M. Peeters,

High-temperature conductance of a two-dimensional superlattice controlled by spin-orbit interaction,

Phys. Rev. B **83**, 115313 (2011).

[III.] P. Földi, **V. Szaszkó-Bogár**, F. M. Peeters,

Spin-orbit interaction controlled properties of two-dimensional superlattices,

Phys. Rev. B **82**, 115302 (2010).

Additional work:

[IV.] **V. Szaszkó-Bogár**, F. M. Peeters, P. Földi,

Oscillating spin-orbit interaction in two-dimensional superlattices: sharp transmission resonances and time-dependent spin-polarized currents,

arXiv:1502.05798 [cond-mat.mes-hall] (2015).

References

[1] E. I. Rashba, Sov. Phys. Solid State **2**, 1109 (1960).

[2] G. Dresselhaus, Phys. Rev. **100**, 580 (1955).

[3] E. A. de Andrada e Silva, G. C. L. Rocca, and F. Bassani, Phys. Rev. B **55**, 16293 (1997).

[4] J. Nitta, T. Akazaki, H. Takayanagi, and T. Enoki, Phys. Rev. Lett. **78**, 1335 (1997).

[5] D. Grundler, Phys. Rev. Lett. **84**, 6074 (2000).

[6] S. Datta and B. Das, Appl. Phys. Lett. **56**, 665 (1990).

[7] D. D. Awschalom, D. Loss, and N. Samarth, *Semiconductor Spintronics and Quantum Computation* (Springer, Berlin, 2002).

[8] I. Žutić, J. Fabian, and S. D. Sarma, Rev. Mod. Phys. **76**, 323 (2004).

[9] L. Esaki and L. L. Chang, Phys. Rev. Lett. **33**, 495 (1974).

[10] T. Koga, J. Nitta, T. Akazaki, and H. Takayanagi, Phys. Rev. Lett. **89**, 046801 (2002).

[11] M. König *et al.*, Phys. Rev. Lett. **96**, 076804 (2006).

[12] S. Datta, *Electronic transport in mesoscopic systems* (Cambridge University Press, Cambridge, 1995).

[13] F. E. Meijer, A. F. Morpurgo, and T. M. Klapwijk, Phys. Rev. B **66**, 033107 (2002).

[14] S. Griffith, Trans. Faraday Soc. **49**, 345 (1953).

[15] C. Kittel, *Quantum Theory of Solids*, 2 ed. (Wiley, New York, 1987).

[16] G. Floquet, Ann. École Norm. Sup. **12**, 46 (1883).

Coauthor's declaration

I hereby certify that I am familiar with the thesis of the applicant **Mr. Viktor Szaszkó-Bogár** entitled Quantum Transport Phenomena Of Two-Dimensional Mesoscopic Structures . Regarding our jointly obtained results that form part of this PhD dissertation, I declare the followings:

The applicant's contribution was prominent in obtaining the following results:

[I.] **V. Szaszkó-Bogár**, P. Földi, F. M. Peeters,

Oscillating spin-orbit interaction as a source of spin-polarized wavepackets in two-terminal nanoscale devices,

J. Phys.: Cond. Matt. **26**, 135302 (2014).

[II.] P. Földi, **V. Szaszkó-Bogár**, F. M. Peeters,

High-temperature conductance of a two-dimensional superlattice controlled by spin-orbit interaction,

Phys. Rev. B **83**, 115313 (2011).

[III.] P. Földi, **V. Szaszkó-Bogár**, F. M. Peeters,

Spin-orbit interaction controlled properties of two-dimensional superlattices,

Phys. Rev. B **82**, 115302 (2010),

I did not and will not use these results in getting an academic research degree.

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