

# **Computer simulations of electronic transport in non-homogeneous nanostructures**

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# 1. Summary of Professional Achievements

## 1.1. Introduction

### 1.1.1. Personal details

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### 1.1.2. Academic degrees

<b>PhD in Physics</b>	2005 AGH University of Science and Technology Kraków Faculty of Physics and Applied Computer Science
<i>Thesis title</i>	<b>Electronic structure of disordered low-dimensional systems</b>
<i>Supervisor</i>	Prof. dr hab. Andrzej Maksymowicz
<i>Reviewers</i>	Prof. dr hab. Tadeusz Balcerzak Prof. dr hab. inż. Janusz Tobała
<b>MSc in Technical Physics</b>	2000 University of Mining and Metallurgy (AGH) Kraków Faculty of Physics and Nuclear Techniques
<i>Thesis title</i>	<b>Modelling of discrete medium flow disturbances in presence of obstacles</b>
<i>Supervisor</i>	Dr inż. Mariusz Kopeć
<i>Reviewer</i>	Prof. dr hab. inż. Witold Dzwinel

### **1.1.3. Employment history in scientific institutions**

**since 10/2006** assistant professor  
Faculty of Physics and Applied Computer Science,  
AGH University of Science and Technology, Kraków, Poland

**10/2005 – 09/2006** teaching and research assistant  
Faculty of Physics and Applied Computer Science,  
AGH University of Science and Technology, Kraków, Poland

## 1.2. Presentation of scientific achievements forming the basis for habilitation procedure

As a scientific achievement within the meaning of Art. 16, par. 2 of the Act of 14 March 2003 “On Academic Degrees and Academic Title and on Degrees and Title in Art” I present a series of eight related publications:

- [H1] B. J. Spisak, M. Wołoszyn. “Nonclassical properties of electronic states of aperiodic chains in a homogeneous electric field”. *Phys. Rev. B* **80** (2009), 035127.
- [H2] M. Wołoszyn, B. J. Spisak. “Multifractal analysis of the electronic states in the Fibonacci superlattice under weak electric fields”. *Eur. Phys. J. B* **85** (2012), 10.
- [H3] B. J. Spisak, M. Wołoszyn, D. Szydłowski. “Dynamical localisation of conduction electrons in one-dimensional disordered systems”. *J. Comput. Electron.* **14** (2015), 916.
- [H4] M. Wołoszyn, J. Adamowski, P. Wójcik, B. J. Spisak. “Periodicity of resonant tunneling current induced by the Stark resonances in semiconductor nanowire”. *J. Appl. Phys.* **114** (2013), 164301.
- [H5] M. Wołoszyn, B. J. Spisak, J. Adamowski, P. Wójcik. “Magnetoresistance anomalies resulting from Stark resonances in semiconductor nanowires with a constriction”. *J. Phys. Condens. Matter* **26** (2014), 325301.
- [H6] M. Wołoszyn, B. J. Spisak, P. Wójcik, J. Adamowski. “Transition from positive to negative magnetoresistance induced by a constriction in semiconductor nanowire”. *Physica E* **83** (2016), 127.
- [H7] M. Wołoszyn, B. J. Spisak. “Stark resonances induced by the exchange–correlation potential in piezoelectric nanowires”. *Phys. Status Solidi RRL* **11** (2017), 1700248.
- [H8] M. Wołoszyn, B. J. Spisak. “Dissipative transport of thermalized electrons through a nanodevice”. *Phys. Rev. B* **96** (2017), 075440.

under a common title:

**“Computer simulations of electronic transport in non-homogeneous nanostructures”.**

### 1.2.1. Introduction

The miniaturization of the electronic circuits and rapidly decreasing extents of devices which are their building blocks makes it necessary to use the quantum description of their operation, as the wave nature of electrons results in phenomena which cannot be neglected in the theoretical description. Examples of such phenomena, found both experimentally and predicted by theoretical calculations, are weak localization and conductance fluctuations, which are related to the quantum interference effects. The theory of quantum transport in nanoscale is therefore one of the most intensively developed fields of modern theoretical physics, and its methods find applications e.g. in nanoelectronics or spintronics. The importance of this approach stems from the fact that understanding of the quantum transport properties allows for development of simulation techniques which can be used for modelling of novel nanodevices and interpretation of experiments. Modelling of the nanodevices using quantum mechanics and advanced numerical methods permits predicting transport properties and investigating the role of many factors including intentional or unintentional defects and inhomogeneities.

Since the fabrication of high-quality multilayer systems has been possible for long time, non-homogeneous systems consisting of any desired sequence of potential wells and barriers can be produced, allowing experimental studies of semiconductor, graphene or photonic superlattices. They may be based also on quasi-periodic sequences,[1, 2, 3, 4] which have many interesting properties, not only purely mathematical but also important for description of physical systems like quasi-crystals[5] (artificially fabricated, but also natural[6]). The sequences of that kind, which are most commonly studied theoretically and experimentally are for example the binary Fibonacci sequence or the Thue–Morse sequence.[7, 8, 9] It is also worth noting that the quasi-periodic systems are usually considered to be intermediate between the ordered and disordered systems, with characteristic features like fractal spectrum and self-similarity.[10, 11]

This type of inhomogeneity can be also fabricated in nanowires, which are important parts of devices having electronic, photonic, energy-conversion, mechanical and other applications.[12] The material inhomogeneity in a nanowire can have a form of layers of different materials embedded in the nanowire, like e.g. in the case of experiments reported for the InAs nanowires with InP barriers,[13, 14] InAs/InSb nanowire field-effect transistors,[15] or GaN/Al<sub>x</sub>Ga<sub>1-x</sub>N nanowire heterostructures.[16] The lack of translational invariance may also result from the presence of an extended defect or deliberately created constriction – an effect that can be created electrostatically by means of the gate-all-around structure, which may be even more desirable for practical applications since it allows electric control of the constriction parameters.[17, 18] In all those cases, presence of a constriction has a profound impact on conductance and other quantities characterizing the transport properties of the considered system.[19, 20, 21] The influence of the magnetic field may also change the transport properties of nanowires with constriction, in particular in terms of possible transition between positive and negative magnetoresistance which was already observed in some other systems, e.g. carbon nanotubes,[22] semiconductor-organic nanocomposites,[23] or InP nanowires.[24] Special attention should be paid to nanodevices made of nitrides, which belong to the class of materials universally used to fabricate nanowires, thanks to their mechanical properties, low density of defects and well-established methods of growth, which makes them useful e.g. as piezoelectric generators[25] or photodetectors.[26] It is typical of them to exhibit a significant internal electric field resulting from the spontaneous polarization and piezoelectric effects.[27] When two different materials, for example GaN and AlGaN, are in contact, there exists a certain charge redistributed on the interface between them, which modifies the profile of the potential energy and influences the electron-electron interactions, which must be taken into account during theoretical and computational studies of their properties.

The publications presented in this summary are devoted both to the quasi-periodic systems, and to the non-homogeneous nanowires of various types. Systems discussed in the first group of the publications ([H1, H2, H3]) are based on random or quasi-periodic sequences defining the positions of scattering centres or alternatively quantum barriers and wells. The remaining publications ([H4, H5, H6, H7, H8]) focus on the analysis of nanodevices with material or



structural inhomogeneities.

## **Purpose of works [H1–H8]**

The aim of the presented research was first of all to examine the effects of the electric field on the global and the local electronic structure of aperiodic (quasi-periodic or disordered) systems, and on the statistical properties of the wavefunctions in such systems or distribution functions in the phase space. Then, in the next stage, I found the transport characteristics of nanowires with material or structural inhomogeneities, starting with one-dimensional models and then using the three-dimensional models and including additional factors, e.g. external magnetic field. Finally, I introduced a more realistic description of the transport phenomena in open systems including scattering processes in contacts.

## **Main results**

The most important results of my research, which I presented in the publications [H1–H8], include:

1. discovery of the periodic properties of the resonant tunnelling current calculated for nanowires with a double-barrier structure that result from the changes of the distance between the source and the drain, or alternatively from the applied source-drain and gate voltages; explaining the origin of those periodic changes in terms of the Stark resonances created in the triangular quantum well created in the spacer region, and proposing an experimental method of observation of such resonances;[H4]  
explaining the role of the exchange-correlation potential for the formation of the Stark resonances in the piezoelectric nanowires, and thus modification of the current flowing through the nanowire and influence on the shot noise;[H7]
2. demonstration of the possibility of anomalous behaviour of magnetoresistance in semiconductor nanowires with constriction, and its relation to the Stark resonances and current peaks; analysis of the influence of the geometric parameters of constriction on the current;[H5]  
calculating the magnetoresistance in the case of spin-dependent magnetotransport in InSb nanowires with constriction, and showing that the sign of the magnetoresistance can be changed depending on the constriction diameter, which is a combined effect of the squeezing of transverse electronic states and the spin Zeeman splitting, and therefore intentionally introduced constriction may serve as a spintronic device;[H6]
3. introduction of improved boundary conditions for the Wigner kinetic equation, allowing more realistic description of transport phenomena including the thermalization of electrons in contacts; testing the influence of the modified boundary conditions on the current-voltage characteristics of a semiconductor nanowire with double-barrier structure;[H8]
4. determining the non-classical properties of quasi-periodic systems based on the Fibonacci and Thue-Morse sequences in terms of the non-classicality parameter, and showing that its maximum values under influence of low electric field coincide with the anti-crossings of the neighbouring energy levels, with changes in the localization and with increasing role of the negative part of the Wigner distribution function;[H1]
5. proving that the electric field does not remove the multifractal character of the wavefunctions calculated for the Fibonacci superlattice, the singularity spectrum remains asymmetric, and the nonlinear character of the dynamics of the energy levels is a consequence of large number of anti-crossings, which correspond to local minima of the Inverse Participation Ratio and maxima of the generalized dimension;[H2]

6. application of the quantum transport equation in the Moyal form to the problem of dynamics of conduction electrons in a disordered system and showing that transport is sub-diffusive due to the weak localization.[H3]

### Methods of calculation

To accomplish the research aims which are listed above, I prepared (as a sole author) computer programs which I then used to execute all calculations described in the presented publications. The calculations were performed using methods of two types. First of them was based on the time-independent Schrödinger equation within the effective mass approximation, which was solved to find the wavefunctions and the corresponding eigenenergies. Depending on the discussed system, the applied model was one- or three-dimensional. In the one-dimensional case, it led to the equation solved by means of the finite difference method for fixed boundary conditions ([H1],[H2]) or as an open system in which the transport properties were analysed ([H4]). On the other hand, when the three-dimensional models of nanowires were involved ([H5],[H6],[H7]), the wavefunctions were assumed to have a quasi-separable form[28] (with  $z$ -axis along the symmetry axis of the nanowire),

$$\psi(\mathbf{r}) = \sum_n \phi_n(z) \chi_n(x, y; z) . \quad (1.1)$$

Within this approximation, the potential energy of conduction electrons is given by the formula

$$U(\mathbf{r}) = U_{\perp}(x, y; z) + U_{\parallel}(z) , \quad (1.2)$$

where  $U_{\perp}(x, y; z)$  is the potential energy of lateral confinement, while the longitudinal potential energy  $U_{\parallel}(z)$  is the sum of several terms corresponding to factors such as the applied potential difference, the electrostatic potential energy, profile of the conduction band bottom, and other depending on the details of the model. As a result of the quasi-separable form of the wavefunctions given by eq. (1.1), the three-dimensional Schrödinger equation is replaced by the equivalent system of two equations, namely,

$$\hat{\mathcal{H}}_{\perp} \chi_n(x, y; z) = E_n^{\perp}(z) \chi_n(x, y; z), \quad (1.3)$$

and

$$\left[ -\frac{\hbar^2}{2} \frac{d}{dz} \frac{1}{m^*_{\parallel}(z)} \frac{d}{dz} + E_n^{\perp}(z) + U_{\parallel}(z) - E \right] \phi_n(z) = \sum_{n'} \Lambda_{nn'}(z) \phi_{n'}(z) , \quad (1.4)$$

where the details of the Hamiltonian  $\hat{\mathcal{H}}_{\perp}$  depend on the assumed model, and the matrix elements  $\Lambda_{nn'}(z)$  represent the coupling between the transverse modes. The form of the above equations is also a consequence of the fact that the material parameters (e.g. the effective mass) inside the nanowire may change along its axis, but do not depend on the  $x$  and  $y$  coordinates. Eq. (1.3) is solved by the variational method using the trial wave function in the form of linear combination of the Gaussians (additionally multiplied by the exponential function of the complex magnetic phase factor if the magnetic field is present). When the transversal energies  $E_n^{\perp}(z)$  are found, eq. (1.4) can be solved using the transfer matrix method or the quantum transmitting boundary method[29] to find the transmission coefficients  $T_n(E)$ , which in turn can be used for example to calculate the current through the analysed device using the Landauer formula,[30]

$$I = \frac{2e}{h} \sum_n \int_0^{\infty} dE T_n(E) [f_S(E) - f_D(E)] , \quad (1.5)$$

where  $f_{S(D)}(E)$  is the Fermi-Dirac distribution function for the electrons in the source (drain), or to calculate the spectral density of the current fluctuations,[31]

$$S = \frac{2e^2}{\pi \hbar} \sum_n \int_0^{\infty} dE T_n(E) [1 - T_n(E)] [f_S(E) - f_D(E)]^2 . \quad (1.6)$$

Schrödinger equation in the form presented above may be also solved together with the Poisson equation. This approach was used in Ref. [H7], where application of the self-consistent Schrödinger-Poisson method allowed including the effects of charge accumulation. For this purpose the Poisson equation was used in the following form,

$$\nabla \cdot [\varepsilon(\mathbf{r})\nabla\varphi(\mathbf{r})] = e[n(\mathbf{r}) - N_D(\mathbf{r})] + \nabla \cdot \mathbf{P}(\mathbf{r}), \quad (1.7)$$

where  $\varphi(\mathbf{r})$  is the electrostatic potential,  $\varepsilon(\mathbf{r})$  is the position-dependent electric permittivity,  $N_D(\mathbf{r})$  is the density of ionized dopants,  $n(\mathbf{r})$  is the local density of the electrons, and  $\mathbf{P}(\mathbf{r})$  is the polarization resulting for example from the existence of the surface charges localized at material interfaces. The effective solution required for the self-consistent procedure in three dimensions with the possibility of defining the boundary condition at any chosen surfaces was possible thanks to the implementation of the multigrid method.

The second class of the used computational methods was devoted to the analysis of the quantum states in the phase space of position and momentum, and was performed in terms of the Wigner distribution function,  $f(x, k, t)$ , where the momentum  $p = \hbar k$  ([H1, H3, H8]). This approach gives a possibility of studying the influence of the quantum effects (e.g. interference, which is ignored when the classical distribution functions and Liouville or Boltzmann equations are used) on the dynamics of charge carriers in terms of the kinetic theory.[32] The Wigner distribution function is defined as the Weyl transform of the density matrix,  $\rho(x, x', t)$ , as

$$f(x, k, t) = \frac{1}{2\pi\hbar} \int d\xi \rho \left( x - \frac{\xi}{2}, x + \frac{\xi}{2}, t \right) e^{-ik\xi}, \quad (1.8)$$

and may take negative values which is not the case of the classical distribution functions. Another advantage of this approach is the fact, that inclusion of scattering is relatively simple within the relaxation time approximation.[33]

When the time-dependent Wigner distribution function is considered, the kinetic equation can be written in the form which is based on the Weyl transform of the equation of motion for the density matrix,

$$\frac{\partial f(x, k, t)}{\partial t} + \frac{\hbar k}{m^*} \frac{\partial f(x, k, t)}{\partial x} + \frac{1}{2\pi i\hbar} \int dk' W(x, k - k') f(x, k', t) = -\frac{f(x, k, t) - f^{\text{eq}}(x, k)}{\tau}, \quad (1.9)$$

where  $f^{\text{eq}}(x, k)$  is the equilibrium Wigner function, and  $\tau$  is the relaxation time corresponding to the scattering processes taken into account. The integral kernel  $W(x, k)$  is defined as

$$W(x, k) = \int dx' \left[ U \left( x + \frac{x'}{2} \right) - U \left( x - \frac{x'}{2} \right) \right] e^{-ikx'}, \quad (1.10)$$

where  $U(x)$  is the potential energy of the conduction electrons. To perform the calculations reported in Ref. [H8], equation (1.9) was solved numerically after discretization on a computational grid chosen so that the minimum momentum resolution was given by the uncertainty principle.[34] Another possibility of finding the time evolution of the Wigner function is based on the split-operator method, adopted to the Moyal form of the kinetic transport equation, and this approach was used in Ref. [H3].

After finding the Wigner function  $f(x, k, t)$ , its marginal distributions can be calculated, e.g., to obtain the electronic density in the coordinate space from the relation

$$n(x, t) = \frac{1}{2\pi} \int dk f(x, k, t). \quad (1.11)$$

Also the current density is available as a result of integration of the found Wigner function according to the formula

$$j(x, t) = \frac{e}{2\pi} \int dk \frac{\hbar k}{m^*} f(x, k, t). \quad (1.12)$$

Additionally for any Hermitian operator  $A$ , its expectation value may be calculated as

$$\langle A(t) \rangle = \int dx dk A_W(x, k) f(x, k, t), \quad (1.13)$$

where  $A_W(x, k)$  is the Weyl transform of the operator.[35] As the electronic states may be represented by the Wigner function, it can be found for a pure state  $|\psi(t)\rangle$  from the relation[36]

$$f(x, k, t) = \int dx' \left\langle x - \frac{x'}{2} \middle| \psi(t) \right\rangle \left\langle \psi(t) \middle| x + \frac{x'}{2} \right\rangle e^{-ikx'}, \quad (1.14)$$

which was used in the calculations described in Ref. [H1].

## 1.2.2. Discussion of the works that make up the series of publications which are the basis of the request for habilitation

[H1] B. J. Spisak, M. Wołoszyn. "Nonclassical properties of electronic states of aperiodic chains in a homogeneous electric field". *Phys. Rev. B* 80 (2009), 035127

First of the presented papers is devoted to the analysis of the electronic states and localization in one-dimensional quasi-periodic systems consisting of quantum wells and barriers. The model assumes a one-particle Hamiltonian, describing a sequence of  $N = 100$  quantum wells in which electrons are influenced by the external electric field  $F$ . Each of the wells is given by the Shaw pseudopotential modified by screening, with parameters chosen to reproduce the ionization energy of copper (the other parameters correspond to material properties of Cu as well), and as a result each well gives one state to the conduction band. Centres of the wells are placed at positions given by one of the two discussed quasi-periodic sequences, namely the Fibonacci binary sequence or the Thue-Morse binary sequence, generated over the set  $0, 1$  using the following substitution rules: (i)  $0 \rightarrow 01$  and  $1 \rightarrow 0$  for the Fibonacci sequence, and (ii)  $0 \rightarrow 01$  and  $1 \rightarrow 10$  for the Thue-Morse sequence.[7, 37] For example, in the case of the binary Fibonacci sequence, application of those rules leads to the sequence  $(0, 1, 0, 0, 1, 0, 1, 0, 0, 1, 0, 0, 1, 0, 1, \dots)$ . Each term of the sequence,  $t_i$ , corresponds to the  $i$ -th site in a simple, periodic lattice;  $t_i = 1$  denotes a site occupied by a well (i.e., existence of the well), and  $t_i = 0$  an empty site.

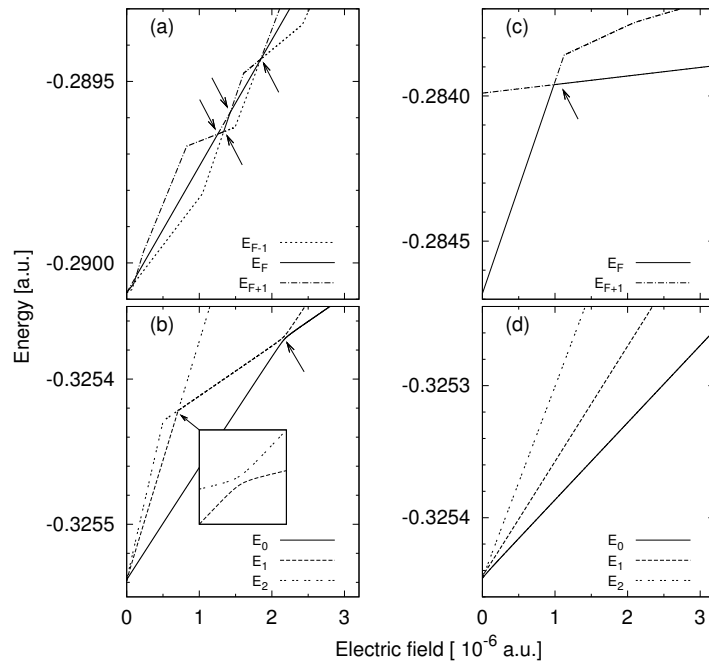


Figure 1.1.: Energies calculated for (a), (b) the Fibonacci sequence and (c), (d) Thue-Morse sequence. (a) and (c) show states at the Fermi level ( $E_F$ ) and directly below and above the Fermi level ( $E_{F-1}$  and  $E_{F+1}$ , respectively). (b) and (d) show states at the bottom of the conduction band. Arrows point to the anti-crossings.[H1]

As it should be expected, the eigenstates of the Hamiltonian form the so-called homogeneous Wannier-Stark ladders when the positions of the wells are periodic. However, the systems based on the quasi-periodic sequences have more complex energy spectra with separate sub-bands. The interplay between the quasi-periodic ordering and the electric field leads in the latter case to the inhomogeneous Wannier-Stark ladders. Closer inspection of the states reveals that slopes of the energy levels as functions of the applied electric field change due to the repulsion between the consecutive levels and occurrence of the so-called anti-crossings, e.g. at the points indicated

by arrows in Figs. 1.1(a), (b), and (c); *a.u.* denotes atomic units of  $\hbar = e = m_e = 1$ .

Detailed analysis of the states, for which the anti-crossings were found, was performed in the phase space. For this purpose, the Wigner distribution function corresponding to the electronic states was calculated using eq. (1.14). Fig. 1.2 shows the Wigner function found for the two lowest states in the system based on the Fibonacci sequence,  $f_0(x, k)$  and  $f_1(x, k)$ , which initially occupy different regions of the phase space. However when the electric field is gradually increased, they are shifted towards the same area, and finally, when the electric field assumes the value corresponding to the anti-crossing between the states  $n = 0$  and  $n = 1$ , they overlap and occupy the same region of the phase space [cf. Figs. 1.2(b) and 1.2(e)]. Further increase of the electric field leads to the state  $n = 0$  occupying the region of the phase space previously taken by the state  $n = 1$  and vice versa.

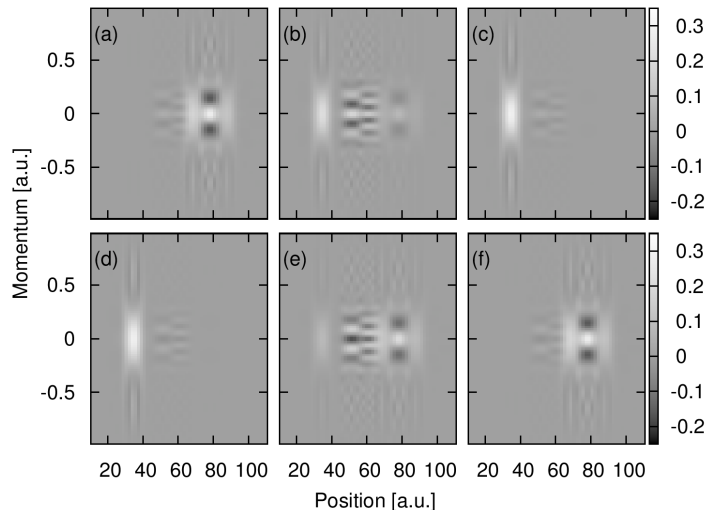


Figure 1.2.: The Wigner function for the system based on the Fibonacci sequence.

(a), (b), (c) – for  $n = 0$ ; (d), (e), (f) – for  $n = 1$ .

Electric field, from left to right, is equal  $1.9, 2.2, 2.5 \times 10^{-6}$  a.u.[H1]

Quantitative analysis of those phenomena is possible via the overlapping integral,  $P_{nm} = 2\pi \int f_n(x, k) f_m(x, k) dx dk$ . For both the quasi-periodic sequences, sharp maxima of  $P_{nm}$  were found at the values of the electric field coinciding with the anti-crossings, while at other values of the electric field  $P_{nm}$  approaches zero since the states are well separated and the quantum interference term disappears. Similar analysis was performed also for the “three-fold” anti-crossings, i.e., at the values of the electric field for which two anti-crossings were found at nearly equal values of the electric field. It was shown that each of these anti-crossings mixes only two neighbouring electronic states, and therefore the previous description applies also to this case.

In order to establish the degree of localization of the considered states in the phase space, the Inverse Participation Ratio (IPR) defined as the integral of the squared Husimi function (i.e., the convolution of the Wigner distribution function and the Gaussian minimizing the uncertainty principle[38]) was calculated. The results presented in Fig. 1.3 illustrate how the electric field modifies the localization of the states near the band bottom and close to the Fermi level. For example in the case of the system based on the Fibonacci sequence, the ground state ( $n = 0$ ) and the first excited state ( $n = 1$ ) exhibit substantial changes of the IPR at the electric field values corresponding to the anti-crossing of those two states [Fig. 1.3(b)]. As it was shown in Fig. 1.2, the first excited state localizes in the region of the phase space previously occupied by the ground state, and vice versa. Hence the values of the  $IPR_n$  are virtually exchanged between those two states: for the electric field below the anti-crossing  $IPR_0 \approx 0.13$  and  $IPR_1 \approx 0.08$ ; above the anti-crossing  $IPR_0 \approx 0.08$  and  $IPR_1 \approx 0.13$ . Results shown in Fig. 1.3 together with the calculations of the expectation values of the squared momentum and position reported in [H1] prove that the changes of localization and shifts of the states due to the electric field

happen in the considered quasi-periodic systems only at the points of anti-crossings, while the IPR values remain almost unchanged far from the anti-crossings, even when the electric field is increasing. Also for the states in the middle of the band, the sharp changes of the IPR can be easily attributed to the anti-crossings, as revealed for example by the comparison of Fig. 1.1(c) and Fig. 1.3(c) presenting results for the Thue-Morse sequence.

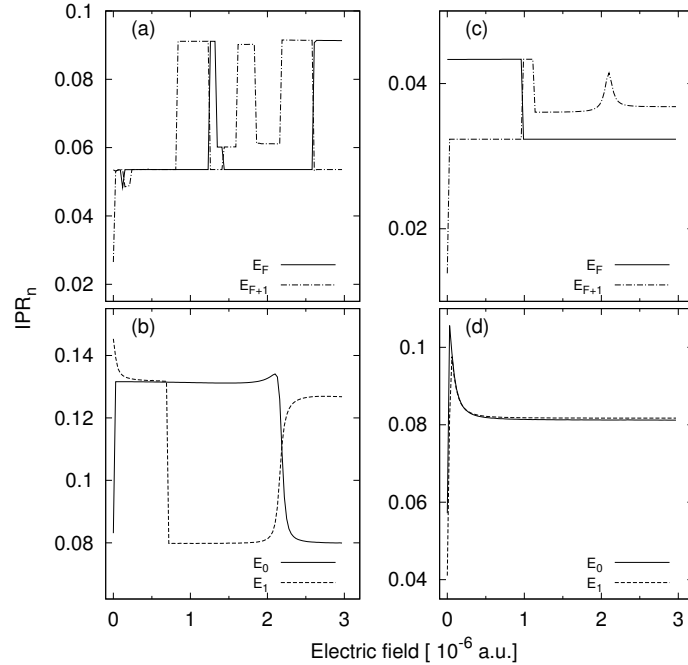


Figure 1.3.: Inverse Participation Ratio ( $IPR_n$ ) (a), (b) for the Fibonacci sequence and (c), (d) for the Thue-Morse sequence.[H1]

In all those cases in which an anti-crossing takes place, the distance between the states on the energy scale is very small. It may suggest that the quantum effects are much more important at such conditions, in particular the effects which are related to quantum interference phenomena. The trace of such effects may be found by analysing the Wigner function in terms of its negative values.[39] When the Wigner function is split into positive and negative parts, they can be integrated separately to find the non-classicality parameter which allows the quantitative description of the non-classical nature of an electronic state. For example, in the case of the ground state in the system based on the Fibonacci sequence, analysis of the non-classicality parameter reveals that its value decreases immediately after the non-zero electric field is turned on. It stays on a constant level up to the electric field at which an anti-crossing takes place, and then rises which stems from the fact that the negative part of the Wigner distribution function becomes significant in both states involved in the anti-crossing. Further increase of the electric field is followed by the decrease of the non-classicality parameter, which proves that anti-crossings are accompanied by maxima of the non-classicality parameter. No such maxima were found in the case of the ground state of the Thue-Morse sequence, which is due to the fact that in this case no anti-crossings were found in the considered range of the electric field because of large separation in the phase space between the ground state and the higher states. It was found that also for the states in the middle of the band the non-classicality parameter rapidly changes its value at the electric fields corresponding to the anti-crossings.

Finally, the uncertainty product  $\sigma_n(x)\sigma_n(k)$  was calculated based on the standard deviations  $\sigma_n^2(x) = \langle x^2 \rangle_n - \langle x \rangle_n^2$  and  $\sigma_n^2(k) = \langle k^2 \rangle_n - \langle k \rangle_n^2$ , which were obtained from the relevant expectation values as given by eq. (1.13). It allows to distinguish between the classical and non-classical states, since for the latter its value is larger than  $1/2$ , which is the case for the states analysed

in [H1]. Similarly as it was found for the non-classicality parameter, also  $\sigma_n(x)\sigma_n(k)$  undergoes rapid changes around the anti-crossings when studied as a function of the applied electric field. This result confirms the non-classical properties of the Wigner functions corresponding to quantum states in the vicinity of an anti-crossing, where the quantum interference phenomena play important role.

**[H2] M. Wołoszyn, B. J. Spisak. “Multifractal analysis of the electronic states in the Fibonacci superlattice under weak electric fields”. *Eur. Phys. J. B* 85 (2012), 10**

The system investigated in this work is a superlattice based on the Fibonacci binary sequence, which consists of a sequence of semiconductor layers made of  $\text{Al}_{0.3}\text{Ga}_{0.7}\text{As}$  and  $\text{GaAs}$ . Different bandgaps of those two materials result in discontinuities of the conduction band profile at the interfaces, and therefore the conduction band potential energy reflects the alternating layers. In [H2] it was modelled as a superposition of the power-exponential functions corresponding to a sequence of  $\text{Al}_{0.3}\text{Ga}_{0.7}\text{As}$  barriers. The positions of barriers are given by the binary Fibonacci sequence generated according to the same procedure as in [H1], where each '1' in the sequence corresponds to one  $\text{Al}_{0.3}\text{Ga}_{0.7}\text{As}$  layer (barrier) and each '0' corresponds to a single  $\text{GaAs}$  layer having the same width as the barrier.

For this system, with the applied external electric field, the time-independent Schrödinger equation was solved to find the wavefunctions  $\psi_n(x)$  and the corresponding eigenenergies  $E_n$ . The total density of states which was then calculated, revealed the presence of minibands manifesting fractal structure at zero electric field. When the electric field was present, the width of the minibands increased and the fractal structure was no longer directly visible. However, in the case of the local density of states, defined as  $\text{LDOS}(x, E) = \sum_n |\psi_n(x)|^2 \delta(E - E_n)$ , the complex structure was found to be preserved even under influence of the electric field, resulting only in the slanted LDOS map when viewed as a function of the position  $x$  and the energy  $E$ .

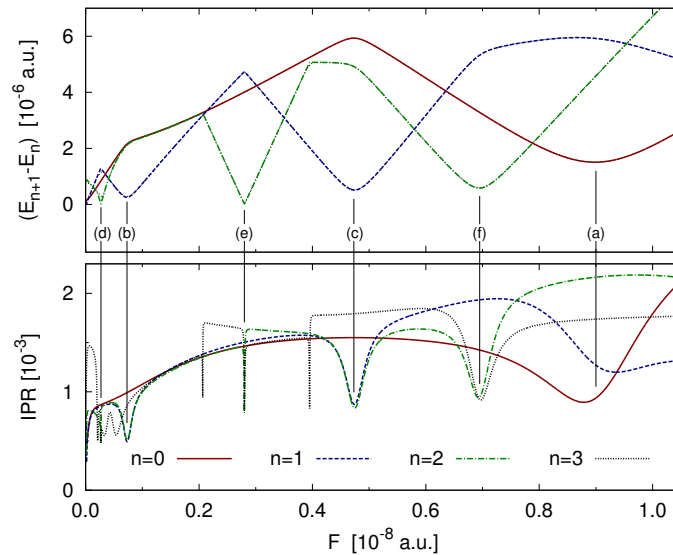


Figure 1.4.: Differences  $(E_{n+1} - E_n)$  between the energies of the four lowest subsequent levels (upper panel) and the corresponding values of the Inverse Participation Ratio (IPR, lower panel) in the case of  $N = 100$  Fibonacci superlattice. Letters (a)-(f) denote the positions of anti-crossings.[H2]

The above-mentioned characteristics of the density of states and the non-uniform structure of the energy spectrum are also related to the presence of the anti-crossings revealed when the eigenenergies are affected by the electric field. Similarly as in the case of the anti-crossings discussed in [H1], the degree of localisation of the wavefunctions changes at such points, which



can be measured in terms of the Inverse Participation Ratio defined in the real space as  $\text{IPR} = \int dx |\psi_n(x)|^4$ . It is also worth noting that while the IPR assumes the lowest values at zero electric field (indicating low degree of localization, as should be expected), its behaviour in the increasing electric field is complex (e.g., for a chosen value of the electric field the highly localized states are neighbouring those with much weaker localisation), unlike for the ordered systems for which the localization degree is simply increasing with the electric field, without much difference between consecutive states. A thorough study of the several of the lowest energy levels was performed to find how they are affected by the external electric field and the coupling to the nearest energy levels. As shown in Fig. 1.4, the distances between the consecutive energy levels,  $(E_{n+1} - E_n)$ , that have minima at the anti-crossings, are smallest at electric fields at which the minima of the IPR also occur. It means that at such points the states become less localised as a result of the coupling between them.

The wavefunctions of one-particle states in quasi-periodic systems tend to be critical, which means that they cannot be classified as extended or localized.[40] Moreover, the electronic states in the quasi-periodic systems are known to reveal the fractal properties, e.g. in terms of the wavefunctions[41, 42] or the transmission coefficient,[43] which was also confirmed experimentally for photonic quasicrystals.[2, 44] The wavefunctions, and in particular the probability density which is calculated from them, can be also regarded in terms of multifractals.[45, 46] For this reason the procedure described in detail in [H2] was used in the considered range of the electric field values to find the singularity strength,  $\alpha_n$ , and the corresponding singularity spectrum,  $f(\alpha_n)$ . [47] The singularity spectrum was found to be strongly asymmetric at zero electric field, and broadening as the electric field increases. During this process the minimal value of the singularity strength,  $\alpha_{min}$ , is basically unchanged, which resembles the properties of disordered systems.[48]

In the next step, the generalized dimension,  $D_n(q) = [f(\alpha_n) - q\alpha_n(q)]/(1 - q)$ , was calculated (for  $q = 2$  it is known as the correlation dimension of the wave function[49]). Its importance stems from the fact that the usual approach to finding the localization length from the exponential spatial decay of wave functions cannot be used because of the strong spatial fluctuations (instead the IPR was analysed, as it is discussed above). The generalized dimension was then used to find the scaling exponent,  $\tau_n(q) = D_n(q)(1 - q)$ , [50] and its non-linear characteristics (as a function of  $q$ ) confirmed the multifractality of the electronic states of the discussed system, which is preserved even when the external electric field is applied (Fig. 1.5). It was also shown that the maxima of  $D_n(q)$  are found for the electric field values matching the anti-crossings and minima of the IPR.

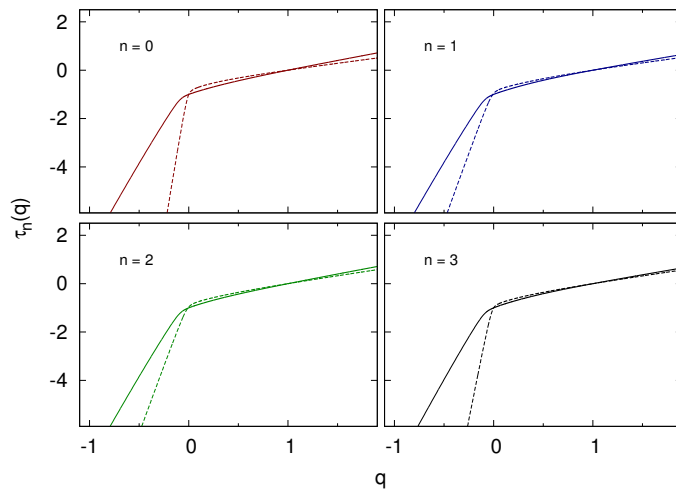


Figure 1.5.: The scaling exponent  $\tau_n(q)$  for the electric field  $F = 0$  (solid line) and  $F = 2 \times 10^{-8}$  a.u. (dashed line) and for states  $n = 0, 1, 2, 3$ . [H2]

The dynamics of the conduction electrons in aperiodic systems was further analysed in [H3]. In this work, the Wigner function formalism was used to simulate the time evolution of the Gaussian wave packets in the phase space, initially centred at the point  $(x_0, p_0)$ , and having parameters typical for the conduction electrons in semiconductor GaAs nanostructures at  $T = 77$  K. The model adopted in this work assumes non-overlapping, short-range scattering potentials, positioned at randomly chosen locations. All the results presented in [H3] were found as a result of averaging over 20 realizations of the disordered system.

The propagation of the Wigner function in terms of its time-dependent evolution was determined by means of the numerical solution with help of the efficient algorithm based on the Moyal form of the Wigner transport equation and application of the Fast Fourier Transform (split-operator method). Thanks to its properties, it was possible to simulate much larger systems (the computational grid consisted of  $N_x = 16384$  by  $N_p = 1024$  points) within longer time periods than in the case of methods based on direct discretization of the Wigner equation. Fig. 1.6 presents the marginal distributions of the Wigner function,  $n(x, t)$  and  $n(p, t)$ , representing the time-dependent probability densities in the coordinate and momentum space, respectively. They show that the maximum of the probability density  $n(x, t)$  remains at the initial position  $x = x_0$  during the simulation, while  $n(p, t)$  reveals two maxima, at  $\pm p_0$ . This result is in agreement with the general theory of weak localization as the multiple scattering processes due to the constructive quantum interference lead to a backscattered peak.[51]

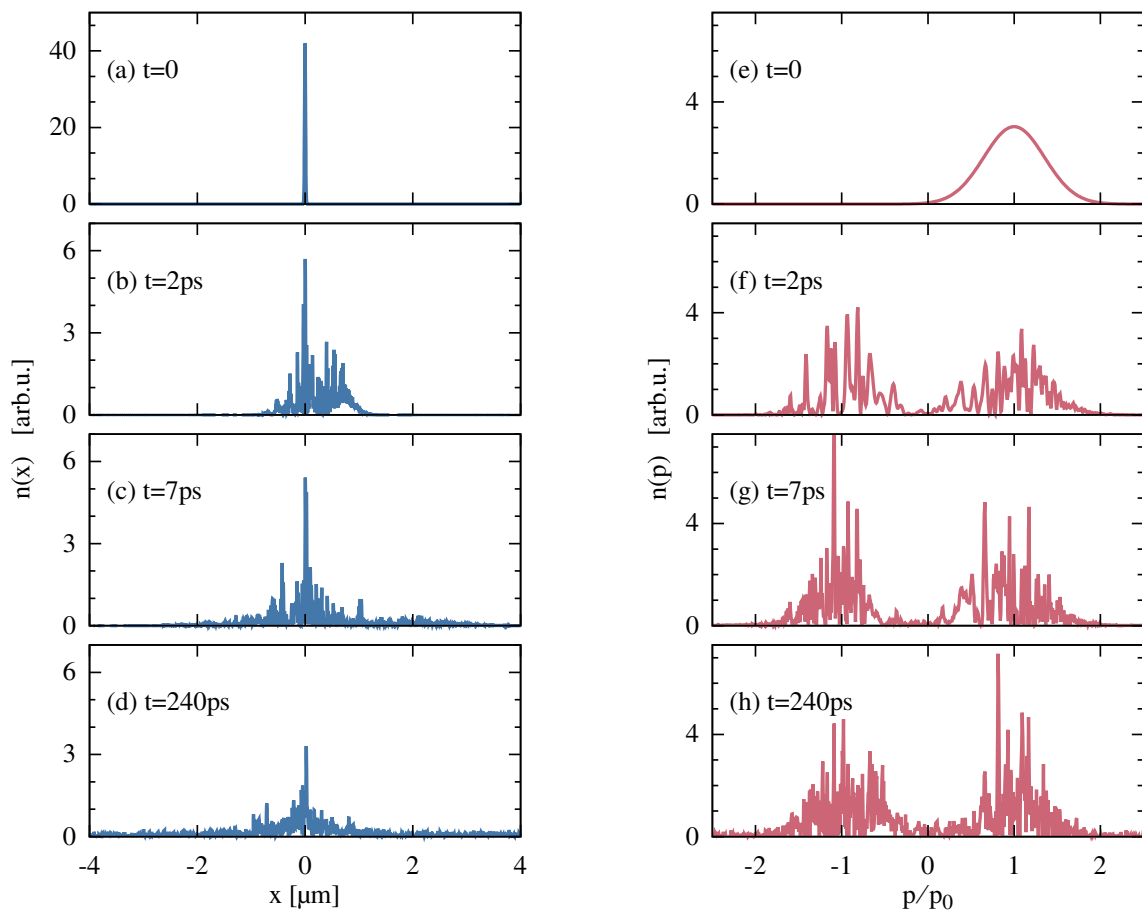


Figure 1.6.: Marginal distributions of the Wigner distribution function in (a-d) coordinate and (e-h) momentum space.[H3]

In order to show that the electronic transport in the analysed disordered system is subdiffusive because of multiple scattering processes which are coherent due to the correlation of momentum, the momentum autocorrelation function,

$$C_p(\Delta t) = \overline{\langle p(t) \rangle \langle p(t + \Delta t) \rangle}, \quad (1.15)$$

was calculated (Fig. 1.7). In (1.15),  $\langle p(t) \rangle$  is the expectation value of the momentum, and the bar symbol denotes the time-average. Since the results exhibited the decay time of the momentum correlations  $\Delta t \approx 9$  ps as nearly three times greater than the scattering time  $\tau = \langle \Delta X \rangle / v_0 \approx 3$  ps (where  $\langle \Delta X \rangle$  is the mean distance between scattering centres, and  $v_0$  is the velocity of the carriers), it was concluded that the successive collisions with the scatterers cannot be treated as independent and that the transport properties reveal non-Markovian properties,[52] while the momentum coherence length  $L_p$  is greater than the mean free path,  $\ell = \langle \Delta X \rangle$ . Additionally, it was shown that the mean-squared displacement,  $\langle x^2(t) \rangle$ , calculated as a function of time fluctuates around a constant value after the initial increase, which also indicates localization. All those results support the conclusion that the slowdown of the electronic transport is a consequence of weak localization and momentum correlations.

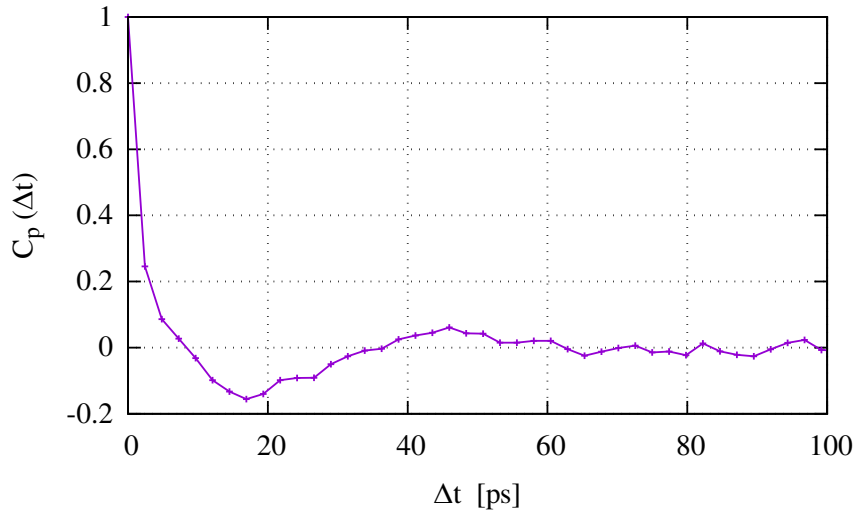


Figure 1.7.: Normalised autocorrelation function of the momentum expectation value. [H3]

[H4] M. Wołoszyn, J. Adamowski, P. Wójcik, B. J. Spisak. “Periodicity of resonant tunneling current induced by the Stark resonances in semiconductor nanowire”. *J. Appl. Phys.* 114 (2013), 164301

The studied system consists of a double-barrier structure contained within a semiconductor nanowire, based on one of the experimental setups for that type of nanodevice with the barriers made of InP placed in an InAs nanowire.[13, 53] The contacts, i.e., the source and the drain electrodes are separated from the barriers by the spacers of width  $s$  each, and the source-drain voltage  $V$  is applied between the electrodes. As this study was devoted to the effects of the geometry and of the applied external voltage, the calculations were performed for the temperature  $T = 0$  which permitted to neglect the scattering effects.

The results presented in [H4] were obtained using the effective mass approximation and the one-dimensional model of the nanowire. The calculated transmission coefficient was used within the Landauer formalism to find the electronic current from eq. (1.5). The resulting current-voltage characteristics reveals a characteristic peak originating from the resonant tunnelling through the central quantum well at the bias voltage of approx. 0.08 V, which is in agreement with experiment.[13] However, its height (maximum current in the peak) varies by a factor of 3 to 5 depending on the spacer width, as shown in Fig. 1.8 (with the largest differences for narrower spacers,  $s < 50$  nm). This repeated switching between the higher (strong) and lower (weak) current peak happens periodically, with the maxima of the current as a function of the spacer width occurring every time  $s$  increases by  $P_s \simeq 28$  nm.

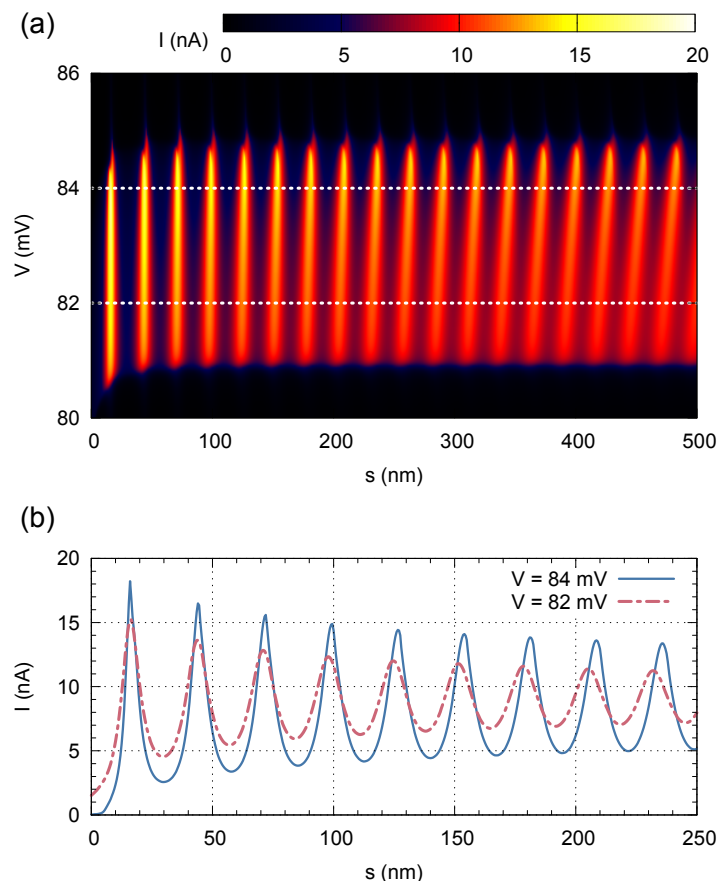


Figure 1.8.: (a) Current  $I$  as a function of the source-drain voltage  $V$  and the spacer width  $s$ . The dotted lines are drawn for  $V = 82$  mV and  $V = 84$  mV. (b) Oscillations of the resonant tunnelling current  $I$  for  $V = 82$  mV and  $V = 84$  mV as a function of  $s$ . [H4]

Explanation of this phenomenon required examining the transmission coefficient and its changes when the spacer width varies at different source-drain voltages, as shown for  $V = 84$  mV in the upper part of Fig. 1.9. The peak of the transmission coefficient considerably changes its width when studied as a function of  $s$ , and becomes much wider for those spacer widths at which the quasi-bound states localized in the triangular quantum well created in the left spacer reach  $E = 0$ . When  $s$  decreases, those states gain energy until they become unbound and go over into the resonance states with  $E > 0$ . The formation of those Stark resonances is periodically repeated, and that way leads to repeatedly increasing width of the transmission coefficient peaks, and in turn to the periodically varying value of the maximum current. The quasi-bound states that become the Stark resonances at certain values of the spacer width  $s$  were found numerically, as shown in the lower part of Fig. 1.9.

A simplified model of the potential energy profile which includes only the triangular quantum well and the left barrier was also constructed in order to find analytical formulas describing the formation of the Stark resonances. Since the slope of the triangular well and its depth are determined by the electric field and the spacer width, the known solution for the energy levels in the infinite triangular well could be used. After using the approximate formula for the  $n$ -th zero of the Airy function it was found that the  $n$ -th quasi-bound state is transformed into the Stark resonance when the following condition is satisfied,

$$\frac{2s_n}{\sqrt{2 + \frac{2b+w}{s_n}}} = \frac{3\pi\hbar}{\sqrt{2meV}} \left( n - \frac{1}{4} \right), \quad (1.16)$$

where  $b$  is the width of each of the barriers, and  $w$  is the width of the central quantum well. The difference between  $s_{n+1}$  and  $s_n$  should correspond to the distance between the strong resonant current peaks, and e.g. for  $V = 84$  mV it was found to be 28.3 nm (for  $n = 1$ ), 27.9 nm (for  $n = 2$ ) or  $P_s \simeq 3\pi\hbar/2\sqrt{meV} = 27.6$  nm when  $s_n \gg 2b + w$ , which means very good agreement with the results shown in Fig. 1.8.

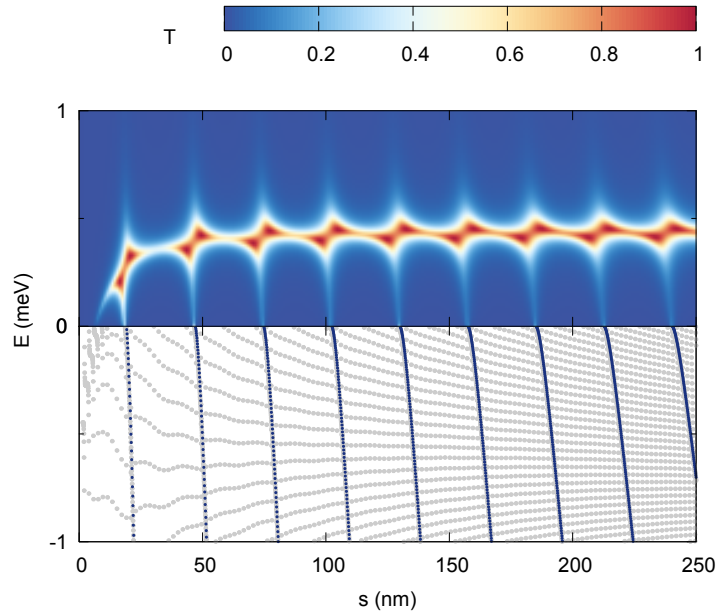


Figure 1.9.: Upper part: Transmission coefficient  $T$  as a function of energy  $E$  and spacer width  $s$ . Lower part: energy levels  $E_n$  of the quasi-bound states as functions of the spacer width  $s$ . Gray dots show the energies calculated for the entire nanodevice (including the contacts) and blue dots show the energy levels of the quasi-bound states localized in the left spacer. The calculations have been performed for  $V = 84$  mV and  $U_G = 0$ . [H4]

Besides the nanowires with different widths of spacers, the case of an additional gate voltage applied in the region of the central well (for example by means of the gate-all-around approach) was also considered. With such arrangement, it was possible to obtain similar results as previously, but for a single nanowire in which the electronic transport was influenced by two independently set voltages: the bias voltage  $V$  applied between the electrodes, and the gate voltage  $V_G$  changing the potential energy inside the central well by  $U_G$ . The latter shifts the quasi-bound states localized in the central quantum well, so that for the fixed geometric parameters ( $s = 1000$  nm) the resonant tunnelling processes resulting in the current peak take place at the bias voltage related to  $U_G$  by the formula  $U_G = 0.515e(V - 85.5\text{mV})$  (note: the prefactor 0.515 is a little bit larger than 0.5 since the applied voltage and the resulting electric field cause slight asymmetry). When both the voltages are changed simultaneously according to this formula, it is possible to follow the maxima of the current corresponding to the resonant tunnelling. As in the case of the varying spacer width, the current maximum oscillates but this time as a function of the applied voltages. The material and geometric parameters used in [H4] led to the results presented in Fig. 1.10, where the strong peaks occur every time the bias voltage is changed by  $P_V \simeq 5.1$  mV together with the change in the  $U_G$  approx. equal 2.6 meV. Analysis of the potential energy profile under such conditions reveals that the mechanism responsible for those changes is of the same nature as in the case of varying spacer width, i.e., it is based on the changing number of the quasi-bound states in the triangular quantum well and the related creation of the Stark resonances, as illustrated in Fig. 1.11.

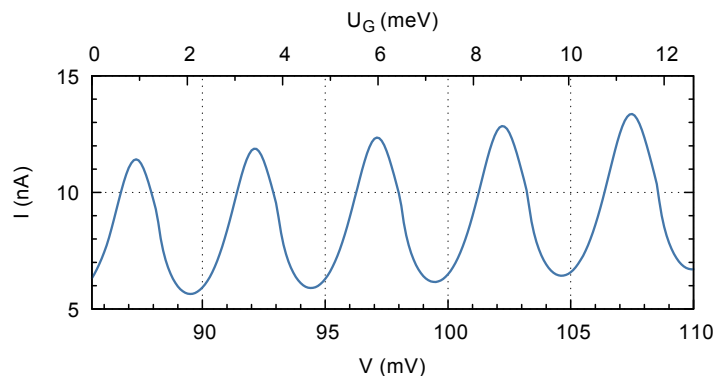


Figure 1.10.: Current  $I$  as a function of the source-drain voltage  $V$  and the gate-voltage induced change of the potential energy  $U_G$  in the central quantum well for the constant spacer width  $s = 1000$  nm. [H4]

The analytical approach discussed above permitted also to find the voltage intervals corresponding to the consecutive strong resonant current peaks as follows,

$$V_{n+1} - V_n = \frac{9\pi^2\hbar^2L}{4mes^3} \left( n + \frac{1}{4} \right), \quad (1.17)$$

where  $L$  is the length of the nanowire. Since  $n$  is the quantum number of the Stark state, eq. (1.17) can be used to identify the Stark resonance state which corresponds to the given strong resonant current peak – for example in the case of results presented in Fig. 1.10, the agreement with the numerical calculations helped to identify the peaks as corresponding to  $n = 37 \div 41$ .

A similar mechanism is observed experimentally in the case of the Quantum Confined Stark Effect.[54] The experiments related to this effect were also performed for similar types of systems as considered in [H4], e.g., for the so-called Quantum Discs responsible for the formation of systems of barriers and quantum wells in GaN/AlN nanowires.[55] The photoemission measurements carried out for them reveal strong shifts of the absorption spectrum due to the applied voltage and dependent on the size and position of the quantum discs inside the nanowire. As in

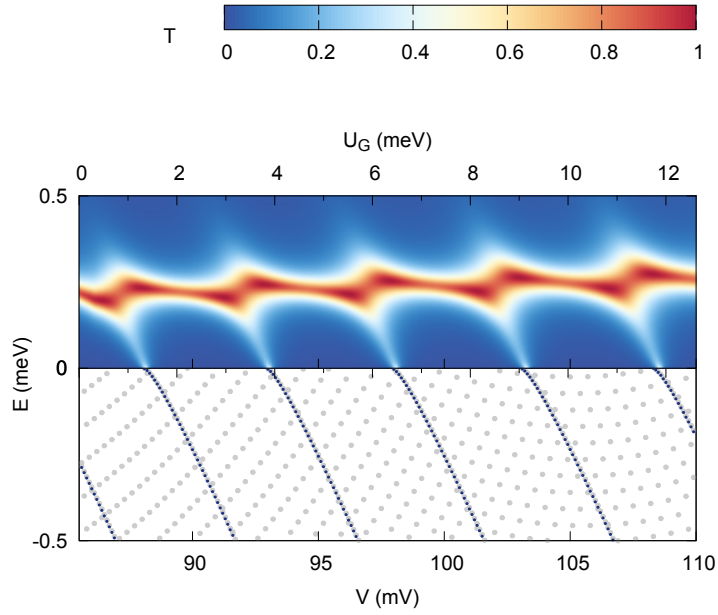


Figure 1.11.: Upper part: Transmission coefficient  $T$  as a function of energy  $E$  and source-drain voltage  $V$  that varies together with the gate voltage. Lower part: energy levels  $E_n$  of the quasi-bound states. [H4]

the case discussed in [H4], it is related to shift of the levels in quantum wells caused by changes in their shape.

**[H5] M. Wołoszyn, B. J. Spisak, J. Adamowski, P. Wójcik. “Magnetoresistance anomalies resulting from Stark resonances in semiconductor nanowires with a constriction”. *J. Phys. Condens. Matter* 26 (2014), 325301**

The Stark resonances discussed in [H4] are expected to emerge in quantum wells created in front of potential barriers, e.g., due to the electric field applied along nanowires. Apart from usage of different materials, the barriers may arise because of the geometric inhomogeneities such as a constriction, introduced intentionally or being simply an extended defect formed during the growth process. Alternatively, a similar effect may be achieved when a side gate or an all-around gate is used to create a constriction-like potential barrier, which could permit control of constriction parameters.

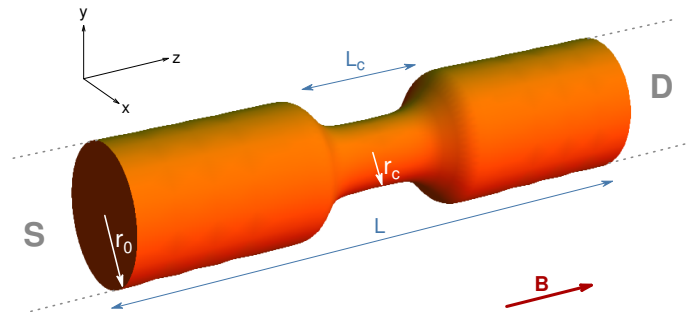


Figure 1.12.: Schematic of the nanowire with constriction:  $r_0$  is the radius of the nanowire outside the constriction,  $r_c$  is the minimal radius of the nanowire in the region of constriction with length  $L_c$ , and  $L$  is the length of the nanowire, i.e., the distance between the source ( $S$ ) and drain ( $D$ ). [H5]

The aim of the calculations presented in [H5] was to analyse how those resonances influence the electronic transport in nanowires with constriction, in particular when the charge carriers are additionally under influence of the magnetic field  $\mathbf{B}$  applied along the axis of the nanowire. For this purpose a three-dimensional model of an InAs nanowire presented schematically in Fig. 1.12 was used, and the calculations were performed within the effective mass approximation, using the following Hamiltonian,

$$\hat{\mathcal{H}} = \frac{1}{2m^*} [\hat{\mathbf{p}} + e\mathbf{A}(\mathbf{r})]^2 + U_{conf}(\mathbf{r}) + eFz, \quad (1.18)$$

where  $\hat{\mathbf{p}}$  is the electron momentum operator,  $\mathbf{A}(\mathbf{r})$  is the vector potential chosen in the symmetric gauge as  $\mathbf{A}(\mathbf{r}) = (\mathbf{B} \times \mathbf{r})/2$ , and  $F$  is the electric field caused by the voltage  $V$  applied between the source and the drain. The confinement potential energy  $U_{conf}(\mathbf{r})$  has the rotational symmetry with respect to the  $z$ -axis, and can be written in the quasi-separable form (1.2), with  $U_{\parallel}(z)$  resulting from the conduction-band bottom, and  $U_{\perp}(x, y; z)$  having the form of finite cylindrical potential well of radius corresponding to the changing radius of the nanowire caused by the presence of the constriction. It was shown that the transverse energy levels,  $E_n^{\perp}(B; z)$ , are similar to the Darwin-Fock levels, whereas the strong influence of the nanowire radius leads to an effective potential barrier along the  $z$ -direction, resulting from the presence of the constriction. Additionally, the increasing magnetic field contributes to a slight increase of the height of this barrier. It was also proved that in the case of the magnetic field applied along the axis of the nanowire, the lowest transverse-state energy levels are independent of the assumed cross-section shape: circular, hexagonal or square, provided that the same cross-sectional area is maintained, and material parameters do not vary in the  $x$ - $y$  plane.

The transmission coefficient was calculated as a function of energy, applied bias voltage and magnetic field, and used to find the electronic current from the Landauer formula (1.5) at

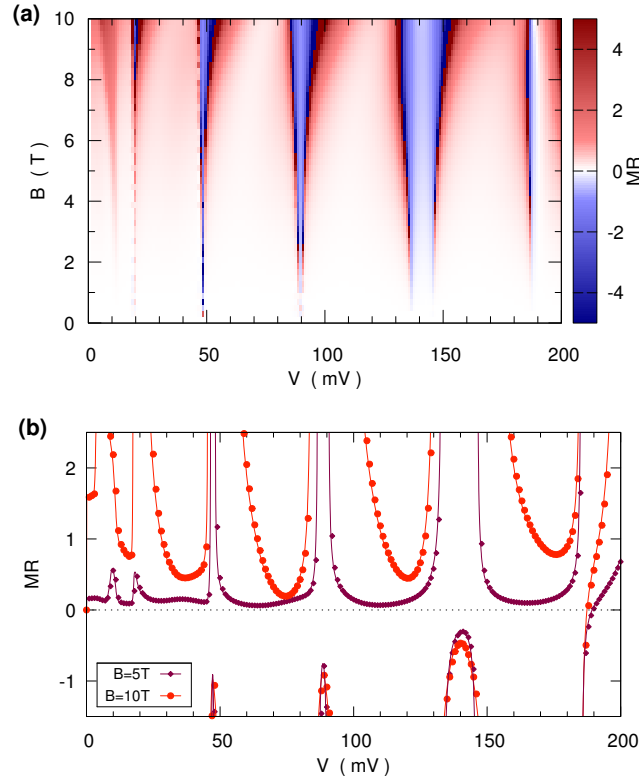


Figure 1.13.: Magnetoresistance MR of the InAs nanowire with the constriction as a function of (a) magnetic field  $B$  and drain-source voltage  $V$ , (b) drain-source voltage  $V$  for  $B = 5$  T and  $B = 10$  T. [H5]



$T = 4$  K. The differential conductance,  $G = \partial I / \partial V$ , revealed a series of maxima and minima, and changes of the sign for any selected value of the magnetic field below 12 T. This oscillatory behaviour of the differential conductance has a direct impact on the magnetoresistance, as demonstrated in Fig. 1.13. The calculated magnetoresistance changes rapidly at certain values of the applied voltage, e.g.  $V \simeq 10, 20, 50, 90$ , and 140 mV, which is a consequence of the singularity transpiring when the differential conductance approaches zero.

The analysis of the current-voltage characteristics obtained for the nanowire with constriction showed that besides the reduction of the current by increasing magnetic field (which is due to the shift of the transverse-state energy levels outside the constriction and thus resultant reduction of the energy transport window), it also reveals distinct current peaks.

Explanation of those phenomena is based on the analysis of the effective potential barrier and the triangular potential well created between the source and the constriction, as shown in Fig. 1.14(a). Although this barrier does not originate from the material differences, but from

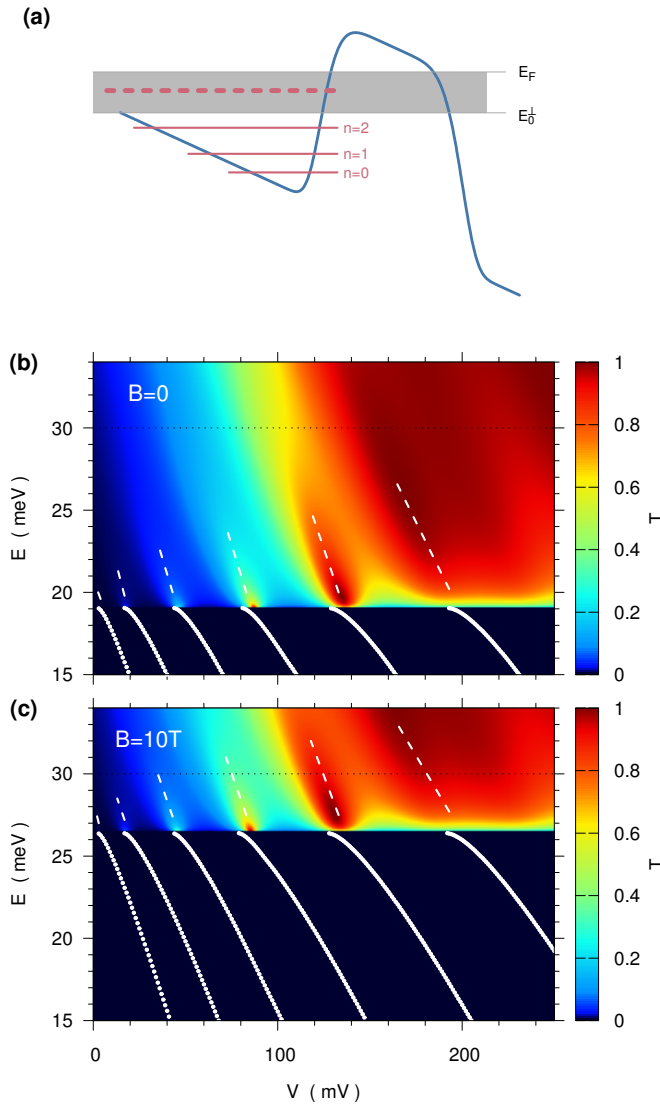


Figure 1.14.: (a) Schematic of potential energy profile  $U_{||}(z)$  (blue curve), energy levels  $E_n^{\parallel}$  (red lines) of the quasi-bound Stark states and the resonant-state energy (broken line) in the transport window. (b) and (c): Transmission coefficient  $T$  as a function of electron energy  $E$  and drain-source voltage  $V$  for (b)  $B = 0$  and (c)  $B = 10$  T; white dashed lines correspond to the energies of Stark resonances, white dots show the energy levels  $E_n^{\parallel}$  of the quasi-bound Stark states. [H5]

the constriction, its role is similar as in the case of the nanowire discussed in [H4]. The quasi-bound states and resonance states (the Stark resonances) which are formed therein, were found to be responsible for the above mentioned properties of the electronic transport characteristics. The enhancements of the transmission coefficient when the quasi-bound states become the resonances, which is presented in Fig. 1.14(b) for  $B = 0$  and in Fig. 1.14(c) for  $B = 10$  T, are therefore induced by the fact that electrons injected from the source traverse the triangular well as Stark resonances (with probability  $\simeq 1$ , unlike the case when no resonance state is within the transport window) and then towards the drain through the barrier created due to the constriction. Except the direct consequence in form of the current peaks at the values of the source-drain voltages at which the Stark resonances are created, this process also influences the differential conductance and the magnetoresistance. Notably, the sign of magnetoresistance is changed because of the corresponding regions of positive and negative differential resistance.

Positions of the current peaks and jumps of magnetoresistance were also analysed in terms of the geometric parameters of the constriction. In particular its radius is of interest since an effect of the same kind may be achieved when instead of varying radius of the nanowire an additional side gate is considered. In such experimental setup, the resulting effective potential barrier can be operated in a continuous manner, which makes it possible to control the magnetoresistance jumps, when also the magnetic field and the source-drain voltage are chosen accordingly to suit that purpose.

**[H6] M. Wołoszyn, B. J. Spisak, P. Wójcik, J. Adamowski. “Transition from positive to negative magnetoresistance induced by a constriction in semiconductor nanowire”. *Physica E* 83 (2016), 127**

The publication [H6] is devoted to the problem of the spin-dependent electronic transport in a nanowire with constriction of the same geometry as shown in Fig. 1.12, and with the magnetic field applied along the axis of the nanowire. It concentrates on the InSb nanowires, in which the phase-coherent transport is observed at low temperatures[56] and the quantization of the conductance was experimentally confirmed.[57] The assumed model describes an InSb nanowire grown in [111] direction, for which the effective mass approximation is used with the  $2 \times 2$  conduction band Hamiltonian as follows,

$$\hat{\mathcal{H}} = \left[ \frac{[\hat{\mathbf{p}} + e\mathbf{A}(\mathbf{r})]^2}{2m^*} + U_{conf}(\mathbf{r}) + eFz \right] \hat{\mathbf{1}} + \hat{\mathcal{H}}_Z . \quad (1.19)$$

Apart from the terms used previously in the Hamiltonian defined in eq. (1.18), it also includes the spin Zeeman splitting term,  $\hat{\mathcal{H}}_Z = g^* \mu_B \mathbf{B} \cdot \hat{\boldsymbol{\sigma}}$ , where  $\mu_B$  is the Bohr magneton,  $g^*$  is the electron effective Landé factor, and  $\hat{\boldsymbol{\sigma}}$  is the vector of the Pauli matrices. In general, the Hamiltonian should also contain the terms describing the spin-orbit interaction, but for a nanowire grown in the [111] direction, the Dresselhaus spin-orbit interaction is absent for momentum along the nanowire.[58] And since both the ends of the nanowire are connected to reflectionless reservoirs (source and drain) with only a small source-drain voltage applied between them, the calculations were performed in the limit of low electric field and also the Rashba term could be neglected. However the intrinsic spin-orbit interaction is included, which is done by means of renormalized electron Landé factor, based on the second-order  $\mathbf{k} \cdot \mathbf{p}$  perturbation theory.[59] When the parabolic approximation of the dispersion relation is assumed, it leads to the following formula for the effective Landé factor,[60]

$$g^* = g \left[ 1 + \left( 1 - \frac{m_0}{m^*} \right) \frac{\Delta_{SO}}{3E_g + 2\Delta_{SO}} \right], \quad (1.20)$$

with  $g$  and  $m_0$  being the Landé factor and the rest mass of free electron in vacuum,  $E_g$  the band gap, and  $\Delta_{SO}$  the spin-orbital splitting. For the considered nanostructure, a modification

to (1.20) was required to include the quantum size effect. Usage of the procedure presented in Ref. [61] resulted in the following relation for the effective Landé factor,

$$g^*(B; z) = g \left[ 1 + \left( 1 - \frac{m_0}{m^*} \right) \frac{\Delta_{SO}}{3[E_g + E_0^\perp(B; z)] + 2\Delta_{SO}} \right]. \quad (1.21)$$

The above formula shows that increase of the nanowire radius leads to the decrease of the effective Landé factor, which approaches the InSb bulk value. The magnetic field, on the other hand, only slightly increases  $g^*$  and this effect is even weaker for smaller radius (when the constriction is narrower). As a consequence, the spin Zeeman splitting is a non-linear function of the magnetic field, affected by the dependence of the electron Landé factor on the diameter due to the constriction in the nanowire.

With all those considerations taken into account, the Pauli equation was solved to find the components of the spinor,  $\psi_\sigma(\mathbf{r})$ , where  $\sigma = \uparrow, \downarrow$ . Owing to the diagonal form of the Pauli equation, each of the spinor components was expanded as given by (1.1), and the potential energy term was decomposed into longitudinal and transversal terms to solve the resulting equations. The matrix elements representing the coupling between the transverse modes could be neglected for the calculations involving only transport through the lowest transverse state, as in the case of the assumed Fermi energy,  $E_F = 50$  meV for which it was verified that  $E_n^\perp > 70$  meV for  $n \geq 1$  in the considered geometry of the nanowire and for magnetic fields not exceeding 8 T. Additionally, because only the lowest transverse state,  $E_0^\perp$ , takes part in transport, and as it was shown in [H5] in such case the shape of the cross-section has negligible influence, the nanowire can be modelled as a cylindrical rod.

The calculations which were performed in the limit of low temperature and low applied source-drain voltage allowed finding the conductance for each of the spin components, and then the conductance and resistance of the nanowire according to the Mott two-current model. Analysis of the obtained results revealed that the transmission coefficient, and therefore also the resistance,

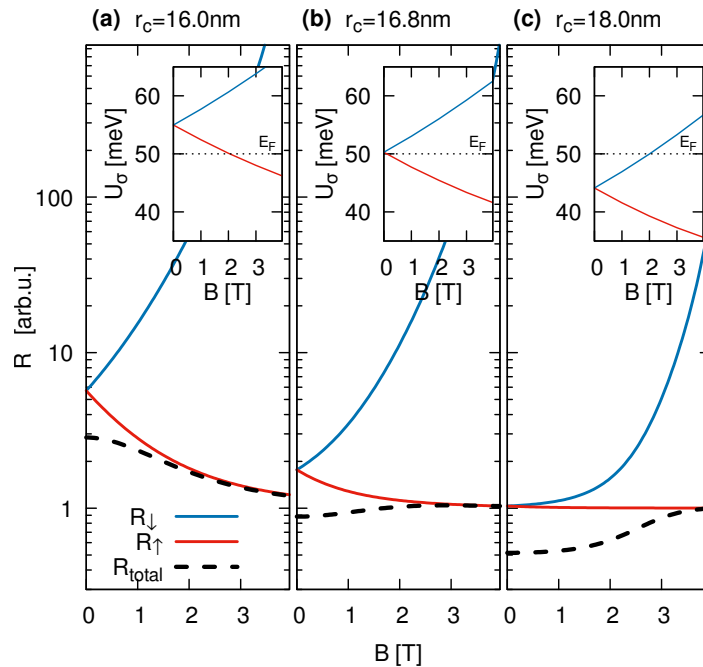


Figure 1.15.: Spin-up ( $R_\uparrow$ , red curves), spin-down ( $R_\downarrow$ , blue curves) and total ( $R_{\text{total}}$ , dashed lines) resistances of the nanowires for three different constriction radii  $r_c$ : (a) 16 nm, (b) 16.8 nm, (c) 18 nm. Insets show the effective heights of barriers at the centres of constrictions, i.e.,  $U_\sigma = E_0^\perp(B; z_0) \pm g^*(B; z_0)\mu_B B$ . [H6]

are strongly influenced by the effective potential barrier due to the constriction. Its height in the middle of the constriction is equal  $U_\sigma(B) = E_0^\perp(B; z_0) \pm g^*(B; z_0)\mu_0 B$ , as presented in the insets of Fig. 1.15. Because at zero magnetic field the barrier height and thus also the transmission coefficient do not depend on the electron spin state, decrease of the constriction radius results in the same changes of the resistance for both spin components. When the magnetic field is applied, the spin degeneracy is lifted which results in decrease of  $U_\uparrow$  and increase of  $U_\downarrow$ .

The outcome of this phenomenon in terms of the resistance is different depending on the geometry of the constriction. If its diameter is only slightly smaller than the diameter of the nanowire outside the constriction, which is the case presented in Fig. 1.15(c), then  $U_\sigma(B=0) < E_F$ . When the magnetic field increases, the spin-up barrier height  $U_\uparrow$  further decreases, and the transmission probability for the spin-up electrons approaches one, which leads to constant, independent of  $B$ , value of  $R_\uparrow$ . On the contrary, the potential barrier for the spin-down electrons,  $U_\downarrow$ , increases with  $B$ , which makes the transmission probability lower and increases  $R_\downarrow$ . The final result is that the total resistance is increasing with magnetic field.

When the constriction is narrower, at  $r_c \simeq 16.8$  nm,  $U_\sigma(B=0) = E_F$  [Fig. 1.15(b)]. In this case, the increase of the magnetic field results in the changes of  $U_\uparrow$  and  $U_\downarrow$  taking place at approximately equal rates, with the former decreasing and the latter increasing. By this reason, the changes of  $R_\downarrow$  and  $R_\uparrow$  compensate, and the total resistance stays at nearly constant level. For even narrower constrictions  $U_\sigma(B=0) > E_F$ , which means that the resistance is much larger than for greater radii  $r_c$ . For increasing  $B$ , the outcome of the changes of  $U_\sigma(B)$  is that  $R_\downarrow$  remains large, while  $R_\uparrow$  becomes smaller and determines the modification of the total resistance which is decreasing, as shown in Fig. 1.15(a).

Those changes of the electronic transport characteristics in the limit of the low applied voltage and due to the applied magnetic field were described in terms of the magnetoresistance. Fig. 1.16

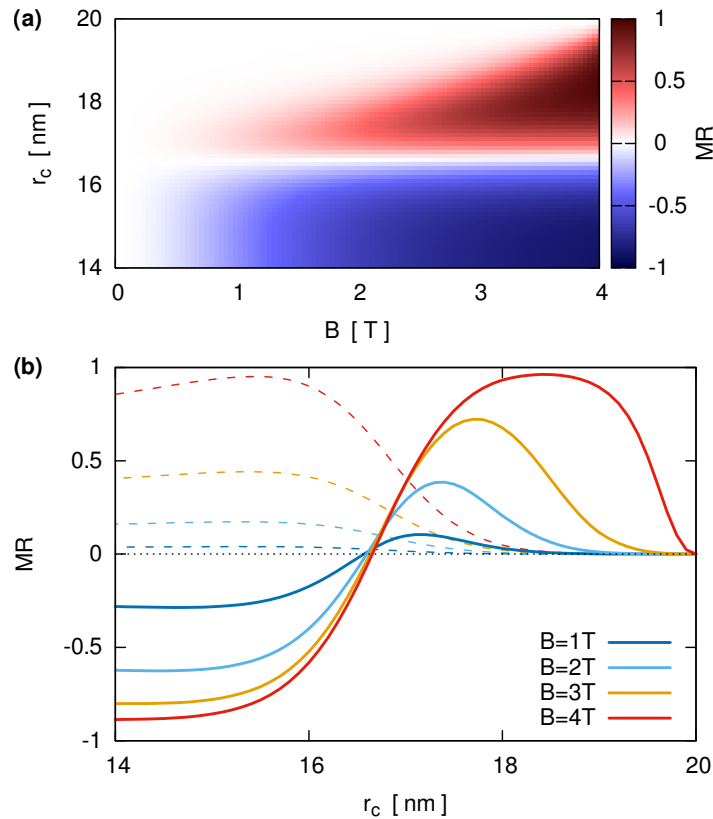


Figure 1.16.: Magnetoresistance as a function of: (a) radius  $r_c$  of the constriction and magnetic field  $B$ , (b) radius  $r_c$  of the constriction [cross sections of (a) at different  $B$ ]; dashed lines correspond to the results obtained when spin of the electrons is neglected).[H6]

shows that the sign of magnetoresistance depends on the radius of the constriction. While the value of the magnetoresistance and its rate of change when the diameter of constriction is modified depend on the applied magnetic field, a common feature is that introduction of the constriction having radius gradually decreased from the nanowire radius (20 nm) results in the increase of positive magnetoresistance up to a maximum depending on the magnetic field. Further narrowing of the constriction decreases the magnetoresistance, which (for the assumed material and geometric parameters) becomes equal zero for  $r_c \simeq 16.8$  nm, independent of the magnetic field. If the constriction has even smaller radius, the magnetoresistance becomes negative and saturates at some constant, magnetic field-dependent level.

The results indicate that InSb nanowires with constriction can be considered as candidates for spintronic nanodevices. Thanks to the intentionally introduced constriction or a ring-shaped gate causing similar effect, they may be useful as spin filters enhancing the spin polarization of the current flowing through the nanowire. In such device the spin filtering operation would be a result of the joint effect of the constriction and the spin Zeeman effect controlled by the magnetic field.

**[H7] M. Wołoszyn, B. J. Spisak. “Stark resonances induced by the exchange–correlation potential in piezoelectric nanowires”. *Phys. Status Solidi RRL* 11 (2017), 1700248**

In [H7], a nanowire made of GaN containing a resonant-tunnelling structure was considered in the limit of low temperature and low applied voltage. The active region consisted of the double-barrier  $\text{Al}_c\text{Ga}_{1-c}\text{N}/\text{GaN}/\text{Al}_c\text{Ga}_{1-c}\text{N}$  structure placed between two GaN spacers and connected to two all-around electrodes, playing roles of the source and the drain [Fig. 1.17(a)]. The length of the left spacer,  $s_L$ , and the concentration  $c$  were the parameters of calculations.

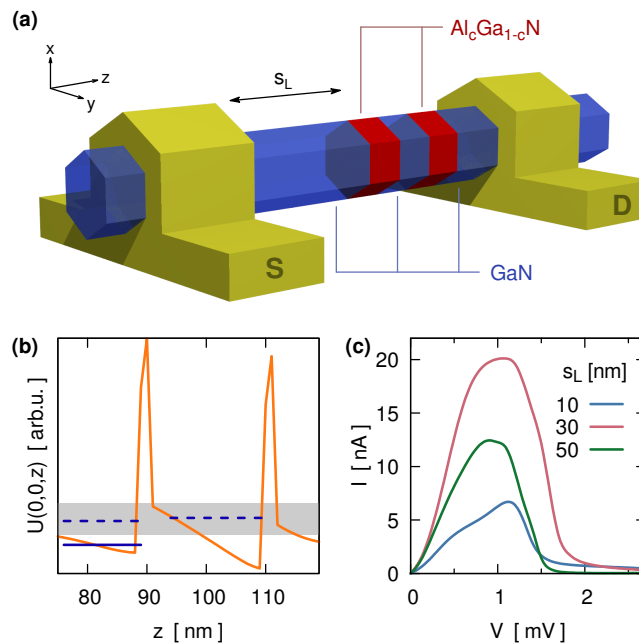


Figure 1.17.: (a) Schematic presentation of the GaN nanowire with two  $\text{Al}_c\text{Ga}_{1-c}\text{N}$  barriers connected to the source (S) and drain (D) electrodes. (b) Self-consistent potential energy along the axis of the nanowire,  $U(0,0,z)$ , in the vicinity of the barriers for the applied voltage  $V = 1$  mV, left spacer length  $s_L = 40$  nm, and concentration  $c = 4$  %. Horizontal solid line denotes the quasi-bound Stark state in the triangular quantum well formed in the left spacer, and the resonant-state energies inside the transport window (grey) are shown with dashed lines. (c) Current-voltage characteristics for different lengths of the left spacer. [H7]

Since the effects of charge accumulation, as well as spontaneous polarization on the interfaces between different materials, were expected to be of great importance, a possibly realistic model accounting for such phenomena and position-dependent material parameters was required. For this purpose the hexagonal cross-section characteristic for wurtzite crystal structure grown in [0001] direction was assumed. The effective one-particle Hamiltonian was used in the form  $\hat{H} = -(\hbar^2/2)\nabla[1/m^*(\mathbf{r})]\nabla + U(\mathbf{r})$ , with the position-dependent electron effective mass. As previously, the potential energy of conduction electrons  $U(\mathbf{r})$  was assumed to have a quasi-separable form given by eq. (1.2). The potential energy included the term resulting from the barriers and the conduction band discontinuity, the electrostatic potential calculated in self-consistent way using the Poisson equation (1.7) with the position-dependent electric permittivity, and the exchange-correlation potential in the form based on Ref. [62].

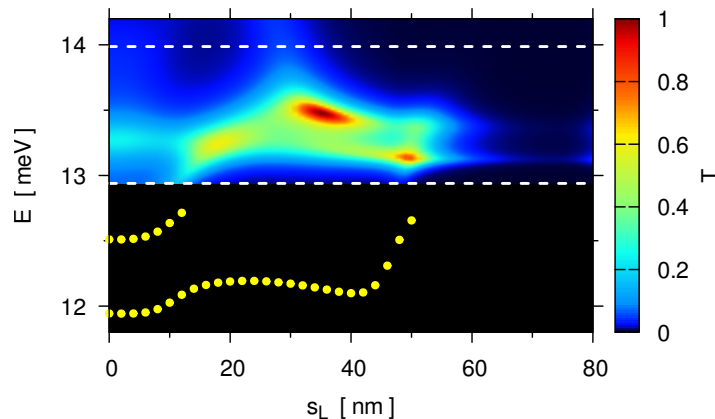


Figure 1.18.: Transmission coefficient,  $T$ , as a function of energy  $E$  and the length of the left spacer,  $s_L$  (upper part) and quasi-bound states localized in the left spacer (lower part), for  $c = 4\%$  and  $V = 1$  mV. White dashed lines indicate the transport window. [H7]

The solution of the three-dimensional Schrödinger-Poisson problem was obtained in self-consistent manner, using the quantum transmitting boundary method[29] to calculate the transmission coefficient  $T(E)$ . Fig. 1.18 shows its dependence on energy and the length of the left spacer  $s_L$  for  $c = 4\%$ , with maxima owing to the overlapping of the effects due to the resonant tunnelling through the central quantum well and due to the quasi-bound states in the triangular well created in the left spacer. Those states (calculated separately for the potential profile resulting from the self-consistent procedure and presented in lower part of Fig. 1.18), after entering the transport window when  $s_L$  is modified become the Stark resonances and therefore increase the value of the transmission coefficient. They also influence the current values calculated from the Landauer formula (1.5): the presented results show that the current flowing through the nanowire has maxima for the spacer lengths corresponding to the Stark resonances, e.g. for  $s_L \simeq 15$  or  $50$  nm, as presented in Fig. 1.19(a). This effect is clearly visible when the concentration  $c$  is sufficient to create a potential well in the spacer with depth which permits for quasi-bound levels. The mechanism responsible for this phenomenon heavily depends on the exchange-correlation interaction. Although the accumulation of charge in the triangular well created by the polarization effects in the left spacer [cf. Fig. 1.17(b)] reduces its depth, this change is compensated by the exchange-correlation potential.

The total current flowing through the nanowire consists of the average current  $I$ , found from the Landauer formula, and the fluctuations due to the noise. For low-temperature limit, the noise may be reduced to the pure shot noise. It is characterized by the Fano factor,  $F = S/(2eI)$ , where  $S$  is the spectral density of the current fluctuations defined in (1.6). Comparison of Fig. 1.19(a) and Fig. 1.19(b) reveals that its local maxima take place for the same values of the concentration and the left spacer length as the maxima of the current. This result indicates

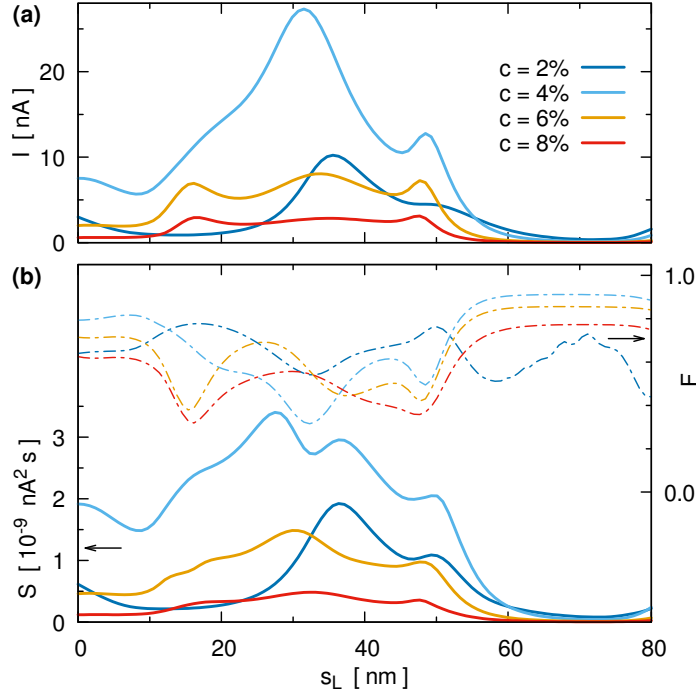


Figure 1.19.: (a) Current  $I$  as a functions of the length of the left spacer,  $s_L$ , and for the concentration  $c = 2, 4, 6$  and  $8$  %. (b) Shot noise  $S$  (solid lines) and Fano factor  $F$  (dashed lines) as functions of  $s_L$ , for various concentrations  $c$ . Both for  $V = 1$  mV. [H7]

that the shot noise, which for the discussed system has values below the values expected for the Poisson distribution of uncorrelated electrons, is further suppressed at the maxima of the current – a characteristic quality of open quantum channels.

**[H8] M. Wołoszyn, B. J. Spisak. “Dissipative transport of thermalized electrons through a nanodevice”. *Phys. Rev. B* 96 (2017), 075440**

Complete theoretical description of transport phenomena in nanodevices should cover not only the wave-like properties of the conduction electrons, but also the exchange of energy with environment and exchange of carriers with the contacts. One of the aspects of this problem was addressed in [H8], where the modified boundary conditions were proposed for the Wigner kinetic equation. They are based on the equilibrium distribution functions which correspond to thermalization of electrons resulting from scattering processes taking place outside of the active region of the nanodevice, and therefore usually are not included in calculations or computer simulations of such devices. The proposed modification takes into account the quality of contacts, and its role for the calculation of the transport characteristics is discussed on the example of a semiconductor nanowire with a double-barrier structure which is a subject of many experimental works (see e.g. Refs.[63, 64, 65]). The active region of the nanowire considered in [H8] consists of two  $\text{Al}_{0.3}\text{Ga}_{0.7}\text{As}$  barriers, the GaAs spacers, and the GaAs quantum well, as shown schematically in Fig. 1.20; the simulation included also the  $n$ -GaAs leads and was performed for the temperature  $T = 77$  K.

Based on the results of Refs. [H5] and [66], an effectively one-dimensional model was assumed to examine the influence of the proposed boundary condition within the framework of the time-independent Wigner kinetic equation (1.9), including the scattering integral in the relaxation time approximation. The usually applied boundary conditions for the Wigner distribution function are a consequence of the free electron model and the distribution of electronic states given

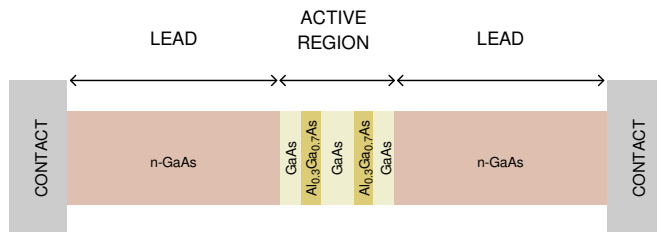


Figure 1.20.: Schematic of the nanowire with active region containing embedded GaAs/Al<sub>0.3</sub>Ga<sub>0.7</sub>As double-barrier structure. [H8]

by the Fermi-Dirac function.[33] As it was indicated in Refs. [67, 68], this kind of separation of the nanosystem and the contacts is not consistent with the non-local character of the quantum mechanics and may produce unphysical results. To overcome those difficulties, a modified form of the boundary conditions proposed in [H8] includes the interaction of carriers with phonons and impurities via the appropriate relaxation times,[69] which assures thermal equilibrium for the conduction electrons.[70] In the case of the considered model, the changed boundary conditions include the scattering processes in contacts, which was achieved by replacing the Fermi-Dirac distribution  $f^{L(R)}(E)$  with its convolution with the Lorentzian  $\delta_\Gamma(E)$ ,

$$f_{eq}^{L(R)}(E(k)) = \int_0^\infty dE \delta_\Gamma(E - E(k)) f^{L(R)}(E), \quad (1.22)$$

where the  $\Gamma$ -parametrized Lorentzian has width proportional to the phase-breaking strength  $\Gamma$ ,

$$\delta_\Gamma(E - E(k)) = \frac{1}{\pi} \frac{\Gamma}{[E - E(k)]^2 + \Gamma^2}, \quad (1.23)$$

which recovers the standard form of the boundary conditions in the limit of  $\Gamma \rightarrow 0$ . On the other hand, the finite value of  $\Gamma$  may result from the influence of the energy exchange between interacting electrons, the interaction between electrons and phonons, or other scattering processes. The value of the parameter  $\Gamma$  may be also defined as the imaginary part of the self-energy, which is in general difficult to find and depends on the details of the electronic structure. However, in the lowest order of the Born approximation, it can be related to the relaxation time for the scattering processes included in (1.22),  $\tau_\Gamma$ , as  $\Gamma = \hbar/(2\tau_\Gamma)$ .

The solution of the Wigner kinetic equation, which was obtained for the potential energy profile including the barriers resulting from the discontinuity of the conduction band and the influence of the bias voltage applied between the contacts, revealed that the implemented boundary conditions decrease the magnitude of the Wigner distribution function when compared to the values obtained in the case of standard boundary condition (i.e., when  $\Gamma = 0$ ), in particular in the regions neighbouring the contacts and for small  $k$ . This change significantly affects the current-voltage characteristics calculated from (1.12), and presented in Fig. 1.21. Its peak, typical for the devices utilizing the effects of resonant tunnelling through the double-barrier structure, has a maximum which strongly depends on the scattering processes taken into consideration.

For the modelled nanodevice, two different cases were examined. In the first of them, the active region of the nanowire (including the leads) was assumed to be dissipationless and thus the dissipation term in the Wigner kinetic equation (1.9) was neglected. The obtained  $I$ - $V$  characteristics [Fig. 1.21(b)] show that the modified boundary condition reduces the peak value of the current by up to about 35% depending on the parameter  $\tau_\Gamma$ . In the second case, the dissipation inside the device was also considered, with the scattering times  $\tau$  assumed in the range estimated on the basis of the effective value of mobility in GaAs,  $\mu = e\tau/m^*$ . The results for  $\tau = 300$  fs and  $\tau = 50$  fs, presented in Figs. 1.21(c) and 1.21(d), respectively, indicate that the peak value of current is further reduced in such cases.



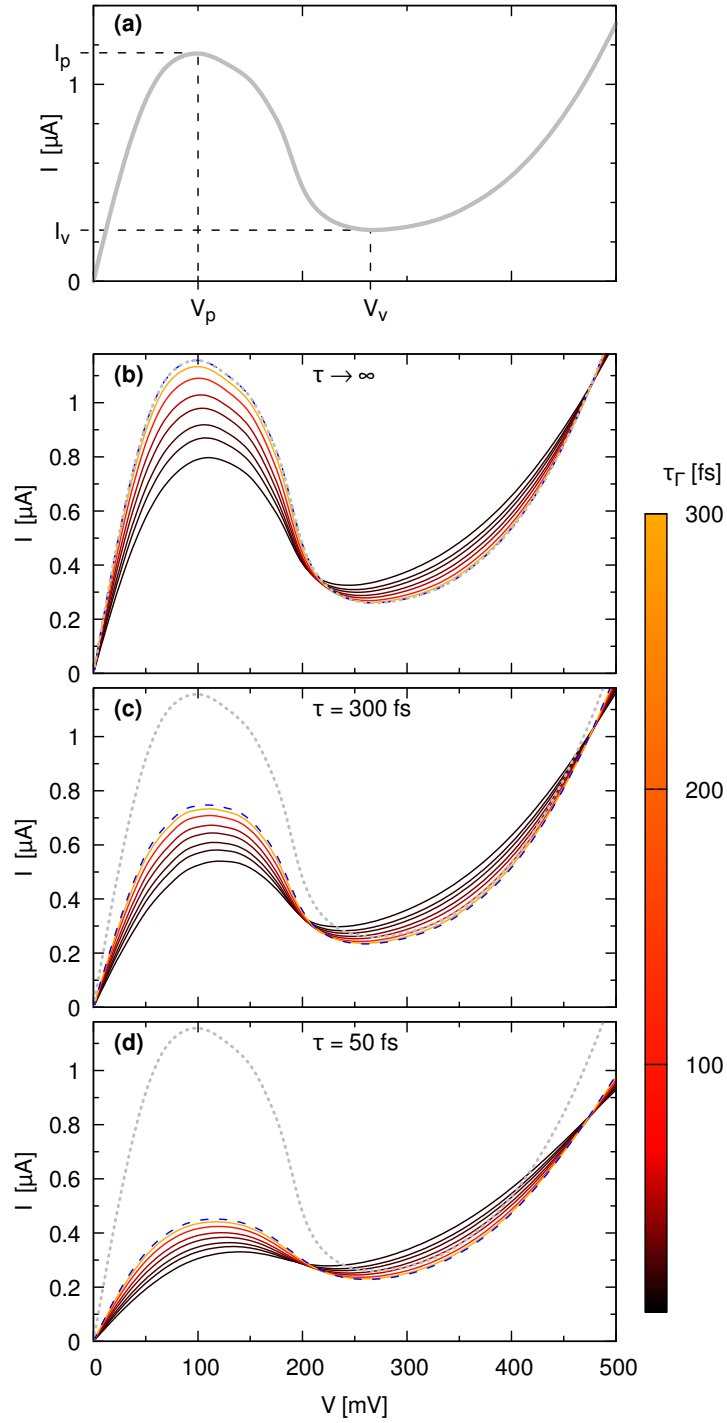


Figure 1.21.: (a) Current-voltage characteristics of the nanowire obtained when no scattering processes of any kind are included, and illustrating the definitions of the peak (valley) voltages,  $V_{p(v)}$ , and currents,  $I_{p(v)}$ . The characteristics calculated for varying relaxation time,  $\tau_\Gamma$ , corresponding to the scattering processes in the contacts, is presented in (b) for the case without scattering inside the nanodevice, (c) for  $\tau = 300$  fs, and (d) for  $\tau = 50$  fs. In (b), (c) and (d), the blue dashed line shows the current for  $\Gamma = 0$ , while the grey dotted line indicates for comparison the characteristics which is shown in (a). [H8]

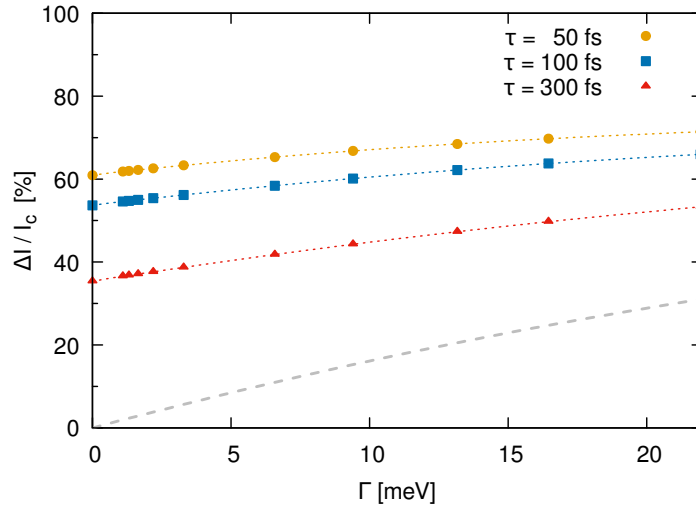


Figure 1.22.: Relative change of the peak current as a function of the parameter  $\Gamma$  for  $\tau = 50, 100, 300$  fs. The dashed grey line corresponds to the case without scattering inside the nanowire. [H8]

The additional analysis performed in terms of the relative change of the peak current (when compared to the dissipationless flow of free electrons) revealed that the thermalization of electrons in the contacts is responsible for the 10÷20% change of the current, depending on the intensity of dissipation inside the nanowire (Fig. 1.22). Also the peak-to-valley ratio of the  $I$ - $V$  characteristics is significantly reduced for positive values of  $\Gamma$ , for example from about 2.5 to 1.5 when  $\Gamma$  changes from zero to 20 meV in the case of  $\tau = 100$  fs. It shows that realistic simulations of the nanodevices should use methods in which it is possible to account not only for the quality of the active region, but also for the quality of contacts and for scattering processes resulting in thermalization of conduction electrons.

### 1.2.3. Summary

The theoretical research of the properties of the non-homogeneous nanostructures presented in publications [H1–H8] allowed me to perform numerical calculations and computer simulations helpful in predicting transport characteristics such as the current-voltage dependencies. In particular, I was able to explain the mechanism of creation of the current oscillations which may result from the Stark resonances in semiconductor nanowires with double-barrier structure, how they influence the magnetoresistance and spin-dependent transport in nanowires with constriction (or all-around gate), and what are the consequences of those phenomena in piezoelectric nanowires. Additionally, I analysed the quasi-periodic systems (including their multifractal and non-classical properties and localization), also in the phase space using the Wigner distribution function formalism. For the latter method, improved boundary conditions allowing more realistic description of transport phenomena were introduced. The possibility of performing such simulations and application of realistic models is of great importance in nanotechnology and spintronics, since it allows to predict the properties of the nanodevices at the initial phase of their design with help of theoretical methods and computer simulations.

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## 1.3. Other scientific achievements

### 1.3.1. Before obtaining the PhD degree

During the PhD studies under supervision of Prof. A.Z. Maksymowicz, I applied the Coherent Potential Approximation (CPA) to perform the calculations of the density of states in binary disordered alloys  $A_xB_{1-x}$ , and to obtain the residual resistivity of such alloys from the complex form of the CPA potential, as a function of concentration  $x$  and for various material parameters.[B4] I also investigated the process of electron localization in disordered molecular wires, in terms of the Inverse Participation Ratio used as a measure of particle localization in disordered medium described by the liquid Kronig-Penney model, and demonstrated the impact of disorder on the ground state of the system.[A36]

For investigation of the disorder and its impact on the density of states in systems with structural disorder, I used a model based on a chain of Dirac's delta potentials in which the increasing level of disorder was introduced to study the deformation of the density of states corresponding the localized states, broadening of the energy bands (exhibited e.g. by amorphous silicon) and influence on the energy gap in the course of the amorphisation process.[B3]

The results of my calculations performed for the PhD thesis allowed finding the localization length, density of states and Inverse Participation Ratio in amorphous systems, and comparing them to the values which I calculated for the periodic and quasi-periodic systems.[A35] Further results allowed me for a detailed study of the formation of bands and gaps, together with comparison of amorphous disorder and disordered binary alloys. [A34]

### 1.3.2. After obtaining the PhD degree

In collaboration with Prof. J. Adamowski, Dr hab. B.J. Spisak, Dr P. Wójcik (Faculty of Physics and Applied Computer Science, AGH) and others, I took part in a project devoted to theoretical studies and numerical simulations of multilayered semiconductor systems. We applied the methods based on the solution of Wigner equation to the triple barrier nanodevice, calculated the current-voltage characteristics, and demonstrated that the triple barrier nanodevice controlled by the gate has a short switching time.[A30] The bistability of the current-voltage characteristics of the triple-barrier resonant tunnelling diode (RTD) and enhancement of the peak-to-valley ratio were explained in terms of the changing potential profile and electron density controlled by the gate potential, as found from the solution of the Wigner-Poisson problem by the self-consistent procedure.[A27] In the following publication,[A26] we found the intrinsic current oscillations (important for design of high-speed electronic circuits) in the asymmetric triple-barrier RTD in two bias voltage ranges, below and above the negative differential resistance region, and explained their origin as resulting from two factors: the negative feedback between the current density and the quasi-bound states in the quantum wells, and the coupling between quasi-bound states in the left quantum well and the quantum well formed in the region of the left contact. Tuning of those terahertz intrinsic oscillations was the topic of the next publication,[A23] in which we demonstrated that the amplitude and frequency of the current oscillations depend on the coupling between the quasi-bound states formed in the quantum wells, which in turn depends on the thickness of the central barrier, allowing adjustment of the amplitude and frequency and application of the asymmetric triple-barrier RTD as a tunable terahertz generator. The wave packet approach to electronic transport in RTD was used to analyse the current oscillations and their decay,[A18] to investigate the influence of the scattering processes on the electronic position-momentum correlations,[A3] and the dynamics of the Gaussian wave packet moving in the double-well potential.[A8]

I participated in the research devoted to the spin-dependent phenomena in resonant-tunnelling devices which may have important implications for design of the spintronic nanodevices, such as spin filters or generators of spin-polarized currents. In the case of the ZnBeSe/ZnMnSe heterostructures, we found two types of hysteresis loops in the non-linear current-voltage char-

acteristics for both spin components of the electronic current (due to accumulation of charge in the central quantum well and the resonant tunnelling through the spin-degenerate quasi-bound state created in the region of the left contact) and we determined the spin polarization of the current reaching high values with possibility of reversing its sign.[A22, A24] The study of the time-dependent electron transport in a paramagnetic RTD under influence of the external magnetic field allowed us to identify and explain the origin of the stable terahertz oscillations of both the spin-up and spin-down current components at constant bias voltage, which may lower the effectiveness of spin filters based on such structures, but also may be used to design generators of the spin polarized current oscillations.[A21] We also investigated the details of the spin filter effect in GaN/GaMnN ferromagnetic RTD without external magnetic field using the self-consistent Wigner-Poisson method, and found that the antiparallel magnetization of the ferromagnetic layers is advantageous for the spin filter operation since it leads to the full spin current polarization at low temperatures and 35% spin polarization of the current at room temperature.[A19]

I was also involved in other research devoted to the spin-dependent phenomena. The differential conductance and the spin polarization of conductance through the metallic nanowire with two magnetic impurities was calculated in the ballistic regime.[A29] In Ref. [A15], we reported on the possibility of all-electrical manipulation of electron spin in semiconductor nanotubes with the spin-orbit interaction related to the radial and axial electric fields. We also showed, that the Rashba spin-orbit coupling in a gate-controlled InAs nanowire may be the basis of the spin transistor operation, and that the gate-voltage induced spin-orbit coupling leads to the oscillations of the source-drain current; the results which were obtained for the case of the partial spin polarization at room temperature were in good agreement with experimental data.[A14] In the next publication related to the problem of spin transistor design ([A12]), we demonstrated the conductance dips in nanowires made of magnetic semiconductors in the helical magnetic field, resulting from the resonant Landau-Zener transitions between the spin-split sub-bands leading to the spin backscattering and possibility of the spin transistor action. The problem of the spin splitting was analysed in Ref. [A11], where the Y-shaped semiconductor nanostructure with a quantum point contact (QPC) placed in a perpendicular magnetic field was used to show that tuning of the QPC potential and the external magnetic field allows almost perfect separation of the spin-polarized currents and application as a spin-splitter in spintronics; additionally such structure may be also used to detect the flow of the spin current. We also showed how the spin currents can be generated and modified in the nanowires with three all-around gates, which can operate as a spin filter controlled by the gates.[A5]

Core-multishell nanowires were the subject of calculations reported in two publications,[A6, A7], in which we analysed the influence of the dimensions of the core and the shells on the transport characteristics in the presence of the surrounding gate and (using the self-consistent approach) the contribution of the accumulated charge and significance of the gate position.

I was cooperating with Prof. D. Stauffer (Institute for Theoretical Physics, University of Cologne) and Prof. K. Kułakowski (Faculty of Physics and Applied Computer Science, AGH) in interdisciplinary research devoted to simulations of opinion dynamics and social networks. We modified Sznajd opinion dynamics model to include the influence of the mass-media advertising, and performed Monte Carlo simulations which allowed us to find the phase transitions in the opinion dynamics, which we also predicted using the mean-field theory.[A33] Investigation of the network model of community by Watts et al. [*Science* **296** (2002), 1302] and consideration of influence of the topology of the social ties on the social collectivity resulted in finding another phase transition, which serves as a parallel to measure the ability of the social system to collective action.[A31]

Marek Wołoszyn

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## 2. Academic activity including didactic achievements, research co-operation and popularization of science

### 2.1. List of publications providing the basis of the achievement

#### A) Title of the achievement

*Computer simulations of electronic transport in non-homogeneous nanostructures*

#### B) Publications providing the basis of the achievement

- [H1] B. J. Spisak, M. Wołoszyn. “Nonclassical properties of electronic states of aperiodic chains in a homogeneous electric field”. *Phys. Rev. B* **80** (2009), 035127  
My contribution to this publication was to take part in the conceptual works, to write all computer programs and execute calculations to solve the Schrödinger equation for the systems based on the quasi-periodic sequences, and then apply methods based on Wigner distribution function. I participated in the analysis of the obtained data, and in preparation of the manuscript. I estimate my contribution to be 50%.
- [H2] M. Wołoszyn, B. J. Spisak. “Multifractal analysis of the electronic states in the Fibonacci superlattice under weak electric fields”. *Eur. Phys. J. B* **85** (2012), 10  
My contribution to this publication was to plan most of the research, and choose the used model of semiconductor superlattice. I wrote the computer program which I later used to perform the calculations resulting in finding the electronic states and their density, and performed analysis of the multifractal properties of those states. I took part in discussion of the obtained results, and prepared most of the manuscript. I estimate my contribution to be 85%.
- [H3] B. J. Spisak, M. Wołoszyn, D. Szydłowski. “Dynamical localisation of conduction electrons in one-dimensional disordered systems”. *J. Comput. Electron.* **14** (2015), 916  
My contribution to this publication was to participate in the development of the research concept and to propose the method of calculation based on the split-operator method. I prepared the computer programs and performed the calculations allowing for the analysis of dynamics of conduction electrons in disordered systems, in terms of the Wigner distribution function. I also took part in discussion of the obtained results, and in preparation of the manuscript. I estimate my contribution to be 45%.
- [H4] M. Wołoszyn, J. Adamowski, P. Wójcik, B. J. Spisak. “Periodicity of resonant tunneling current induced by the Stark resonances in semiconductor nanowire”. *J. Appl. Phys.* **114** (2013), 164301  
My contribution to this publication was to participate in the conceptual works and to plan the calculations. I implemented all computer programs and executed simulations of a semiconductor nanowire with double-barrier structure. Based on the preliminary results, I proposed further studies which allowed finding the periodic behaviour of the current which can be caused either by varying geometric parameters, or by changes in the applied source-drain and gate voltages. I also prepared the simplified model, for which I performed analytical calculations which helped to explain the basics of the described phenomenon. I

took part in discussion of the obtained results, and I prepared most of the manuscript. I estimate my contribution to be 85%.

- [H5] M. Wołoszyn, B. J. Spisak, J. Adamowski, P. Wójcik. “Magnetoresistance anomalies resulting from Stark resonances in semiconductor nanowires with a constriction”. *J. Phys. Condens. Matter* **26** (2014), 325301

My contribution to this publication was to participate in planning of the research and developing the theoretical model applicable to nanowires with constriction in the magnetic field. I wrote the computer programs which I used to execute the calculations, and performed the analysis of the results to provide the explanation of the changes in the magnetoresistance and the electronic current. I also prepared most of the manuscript. I estimate my contribution to be 75%.

- [H6] M. Wołoszyn, B. J. Spisak, P. Wójcik, J. Adamowski. “Transition from positive to negative magnetoresistance induced by a constriction in semiconductor nanowire”. *Physica E* **83** (2016), 127

My contribution to this publication was to participate in planning of the research, and adapting the previously used models and computational techniques to the problem of spin-dependent electronic transport in magnetic field. I wrote all computer programs and used them to obtain all the results presented in this paper. I participated in interpretation of the results, and formulation of explanation of the changes of the magnetoresistance. I prepared a substantial part of the manuscript. I estimate my contribution to be 75%.

- [H7] M. Wołoszyn, B. J. Spisak. “Stark resonances induced by the exchange–correlation potential in piezoelectric nanowires”. *Phys. Status Solidi RRL* **11** (2017), 1700248

My contribution to this publication was to take part in the planning of the project, and defining the used theoretical model. I was the author of the computer programs and I executed all the calculations. I participated in discussion and interpretation of the results, and I prepared most of the manuscript of the publication. I estimate my contribution to be 85%.

- [H8] M. Wołoszyn, B. J. Spisak. “Dissipative transport of thermalized electrons through a nanodevice”. *Phys. Rev. B* **96** (2017), 075440

My contribution to this publication was to participate in the conceptual works which led to the proposal of the modified boundary condition. I implemented the computer program and performed all the numerical calculations resulting in the presented current–voltage characteristics. I took part in discussion of the obtained results, and I prepared a substantial part of the manuscript. I estimate my contribution to be 80%.

## 2.2. List of other scientific publications and bibliometric indicators

### A) Publications in journals tracked by the Journal Citation Report (JCR)

- U. Kaczor, M. Wołoszyn, B. J. Spisak. “Phase-space approach to the position-momentum correlations of the conduction electron states in a double-barrier resonant nanosystem”. *Acta Phys. Pol. A* **132** (2017), 106

My contribution to this publication was to take part in planning of the research. I also wrote the computer program which was used by the first author to execute the calculations, and participated in discussion of the results and preparation of the manuscript. I estimate my contribution to be 35%.

- M. Wołoszyn, B. J. Spisak, P. Wójcik, J. Adamowski. “Spin conductance of nanowires with double coupled quantum dots”. *Acta Phys. Pol. A* **129** (2016), A–114

My contribution to this publication was to participate in planning of the research, and to prepare the computer programs used to simulate the operation of the nanodevice. I

- executed all the calculations, and took part in discussion and interpretation of the results. I wrote the preliminary version of the manuscript. I estimate my contribution to be 80%.
3. T. Palutkiewicz, M. Wołoszyn, P. Wójcik, B. J. Spisak. “Transport characteristics of gated core-multishell nanowires: self-consistent approach”. *Acta Phys. Pol. A* **130** (2016), 1190  
My contribution to this publication was to participate in conceptual works, and to assist in preparation of the computational procedures. I also took part in discussion of the obtained results, and preparation of the manuscript. I estimate my contribution to be 25%.
  4. T. Palutkiewicz, M. Wołoszyn, P. Wójcik, J. Adamowski, B. J. Spisak. “Influence of geometrical parameters on the transport characteristics of gated core-multishell nanowires”. *Acta Phys. Pol. A* **129** (2016), A–111  
My contribution to this publication was to take part in planning of the calculations, discussion of the results and preparation of the manuscript. I estimate my contribution to be 20%.
  5. U. Kaczor, B. Klimas, D. Szydłowski, M. Wołoszyn, B. J. Spisak. “Phase-space description of the coherent state dynamics in a small one-dimensional system”. *Open Phys.* **14** (2016), 354  
My contribution to this publication was to participate in conceptual works, and to help in writing the computer programs using the split operator method. I also took part in analysis of the results, and in preparation of the manuscript. I estimate my contribution to be 15%.
  6. B. J. Spisak, M. Wołoszyn. “Quantum kinetic theory of the 2kF scattering mechanism for three-dimensional structurally disordered systems in the Ioffe-Regel limit”. *Acta Phys. Pol. A* **128** (2015), 213  
My contribution to this publication was to perform part of the analytical calculations and to participate in the discussion of the results. I also took part in preparation of the manuscript. I estimate my contribution to be 25%.
  7. P. Wójcik, J. Adamowski, M. Wołoszyn, B. J. Spisak. “Spin splitting generated in a Y-shaped semiconductor nanostructure with a quantum point contact”. *J. Appl. Phys.* **118**, 014302 (2015), 014302  
My contribution to this publication was to participate in conceptual works, in the discussion of the results of numerical calculations, and in preparation of the manuscript. I estimate my contribution to be 10%.
  8. P. Wójcik, J. Adamowski, M. Wołoszyn, B. J. Spisak. “Resonant Landau–Zener transitions in a helical magnetic field”. *Semicond. Sci. Technol.* **30** (2015), 065007  
My contribution to this publication was to participate in conceptual works, and in the analysis of the results and preparation of the manuscript. I estimate my contribution to be 10%.
  9. P. Wójcik, J. Adamowski, B. J. Spisak, M. Wołoszyn. “Spin transistor operation driven by the Rashba spin-orbit coupling in the gated nanowire”. *J. Appl. Phys.* **115**, 104310 (2014), 104310  
My contribution to this publication was to take part in planning of the research, in the discussion of the results and their analysis versus the experimental data, and in preparation of the manuscript. I estimate my contribution to be 10%.
  10. P. Wójcik, J. Adamowski, M. Wołoszyn, B. J. Spisak. “All-electrical manipulation of electron spin in a semiconductor nanotube”. *Physica E* **59** (2014), 19  
My contribution to this publication was to take part in planning of the research, and in the analysis of the results and preparation of the manuscript. I estimate my contribution to be 15%.

11. B. J. Spisak, M. Wołoszyn, P. Wójcik. “Influence of dephasing and geometrical parameters on quantum correction to dc conductance of cylindrical nanowires”. *Acta Phys. Pol. A* **124** (2013), 838  
My contribution to this publication was to use the obtained analytical formula to execute numerical calculations which resulted in the presented examples of the corrections to the DC conductance. I also took part in the discussion of the results, and preparation of the manuscript. I estimate my contribution to be 30%.
12. D. Szydłowski, M. Wołoszyn, B. J. Spisak. “Phase-space description of wave packet approach to electronic transport in nanoscale systems”. *Semicond. Sci. Technol.* **28** (2013), 105022  
My contribution to this publication was to participate in conceptual works, and in preparation of computer programs used for the calculations. I also worked out the results and verified their correctness, took part in their analysis and in preparation of the manuscript. I estimate my contribution to be 35%.
13. P. Wójcik, J. Adamowski, M. Wołoszyn, B. J. Spisak. “Spin filter effect at room temperature in GaN/GaMnN ferromagnetic resonant tunnelling diode”. *Appl. Phys. Lett.* **102**, 242411 (2013), 242411  
My contribution to this publication was to participate in planning of the research, and in discussion and interpretation of the results of the calculations. I participated in preparation of the manuscript. I estimate my contribution to be 15%.
14. P. Wójcik, J. Adamowski, M. Wołoszyn, B. J. Spisak. “Intrinsic oscillations of spin current polarization in a paramagnetic resonant tunneling diode”. *Phys. Rev. B* **86** (2012), 165318  
My contribution to this publication was to participate in planning of the research and in discussion of the results of numerical calculations. I also took part in preparation of the manuscript of the publication. I estimate my contribution to be 15%.
15. P. Wójcik, B. J. Spisak, M. Wołoszyn, J. Adamowski. “Hysteresis loops of spin-dependent electronic current in a paramagnetic resonant tunnelling diode”. *Semicond. Sci. Technol.* **27** (2012), 115004  
My contribution to this publication was to participate in conceptual works, and in the analysis of the obtained data. I participated in preparation of the manuscript. I estimate my contribution to be 15%.
16. P. Wójcik, B. J. Spisak, M. Wołoszyn, J. Adamowski. “Tuning of terahertz intrinsic oscillations in asymmetric triple-barrier resonant tunneling diodes”. *J. Appl. Phys.* **111**, 124310 (2012), 124310  
My contribution to this publication was to participate in conceptual works, and in discussion and interpretation of the results. I also took part in preparation of the manuscript. I estimate my contribution to be 15%.
17. P. Wójcik, B. J. Spisak, M. Wołoszyn, J. Adamowski. “Simulation of spin-dependent electronic transport through resonant tunnelling diode with paramagnetic quantum well”. *Acta Phys. Pol. A* **119** (2011), 648  
My contribution to this publication was to participate in planning of the research, discussion of the results and in preparation of the manuscript. I estimate my contribution to be 10%.
18. P. Wójcik, A. Naylor, M. Wołoszyn, B. Hickey, B. J. Spisak, J. Adamowski. “Influence of barrier width on spin-polarisation measured by point contact Andreev reflection”. *J. Supercond. Nov. Magn.* **24** (2011), 939  
My contribution to this publication was to participate in discussion of the results and preparation of the manuscript. I estimate my contribution to be 5%.

19. P. Wójcik, B. J. Spisak, M. Wołoszyn, J. Adamowski. “Intrinsic current oscillations in an asymmetric triple-barrier resonant tunnelling diode”. *Semicond. Sci. Technol.* **25** (2010), 125012  
My contribution to this publication was to take part in conceptual works, to prepare the computer program and to execute calculations of the energies of quasi-bound states. I also took part in the analysis and interpretation of the results, and in preparation of the manuscript. I estimate my contribution to be 20%.
20. P. Wójcik, B. J. Spisak, M. Wołoszyn, J. Adamowski. “Self-consistent Wigner distribution function study of gate-voltage controlled triple-barrier resonant tunnelling diode”. *Semicond. Sci. Technol.* **24** (2009), 095012  
My contribution to this publication was to participate in planning the calculations, and to take part in discussion of the results, as well as in preparation of the manuscript. I estimate my contribution to be 15%.
21. B. J. Spisak, M. Wołoszyn, A. Paja. “Spin-dependent transport through metallic system with magnetic impurities”. *Acta Phys. Pol. A* **115** (2009), 266  
My contribution to this publication was to participate in planning of the research and defining the theoretical model. I prepared the computer program used for all the calculations, and executed them. I participated in preparation of the manuscript. I estimate my contribution to be 45%.
22. P. Wójcik, B. J. Spisak, M. Wołoszyn, J. Adamowski. “Application of non-classical distribution function to the transport properties of semiconductor nanodevices”. *Acta Phys. Pol. A* **114** (2008), 1431  
My contribution to this publication was to participate in conceptual works, and in discussion of the results and preparation of the manuscript. I estimate my contribution to be 10%.
23. M. Wołoszyn, D. Stauffer, K. Kułakowski. “Order-disorder phase transition in a cliquy social network”. *Eur. Phys. J. B* **57** (2007), 331  
My contribution to this publication was to write the computer programs, and apply them to perform all the simulations. I also took part in discussion of the results and preparation of the manuscript. I estimate my contribution to be 65%.
24. B. J. Spisak, M. Wołoszyn. “One-dimensional aperiodic systems in phase space”. *Acta Phys. Pol. B* **38** (2007), 1951  
My contribution to this publication was to participate in planning of the research, to prepare the computer programs used in all the calculations, and to perform them. I participated in analysing the obtained results, and in preparation of the manuscript. I estimate my contribution to be 50%.
25. M. Wołoszyn, D. Stauffer, K. Kułakowski. “Phase transitions in Nowak-Sznajd opinion dynamics”. *Physica A* **378** (2007), 453  
My contribution to this publication was to prepare the computer programs which I used to perform all the simulations. I also participated in the discussion of results and in preparation of the manuscript. I estimate my contribution to be 60%.
26. A. Z. Maksymowicz, M. Wołoszyn. “Density of states in structurally disordered 1D chains of atoms”. *J. Non-Cryst. Solids* **352** (2006), 4200  
My contribution to this publication was to participate in planning of the research. I prepared the programs used in all calculations, and performed them. I also participated in preparation of the manuscript. I estimate my contribution to be 50%.
27. M. Wołoszyn, B. J. Spisak, A. Z. Maksymowicz. “Phase space description of localization in disordered one-dimensional systems”. *Acta Phys. Pol. A* **110** (2006), 523

My contribution to this publication was to take part in conceptual works and in defining the theoretical model. I implemented the computer program, and performed all the calculations. I took part in analysis of the results of calculations, and in preparation of the manuscript. I estimate my contribution to be 65%.

28. M. Wołoszyn, B. J. Spisak. “On the localization of electrons in disordered molecular wires”. *Materials Science (Poland)* **22** (2004), 545

My contribution to this publication was to participate in planning of the research. I authored the computer program which I used to perform all calculations which allowed obtaining results presented in the publication. I also took part in discussion of the results, and in preparation of the manuscript. I estimate my contribution to be 70%.

## **B) Inventions and other objects of industrial property which are granted patent protection and were demonstrated at national or international exhibitions**

## **C) Monographs, academic publications in international or national journals that are not tracked by the JCR database**

1. T. Palutkiewicz, M. Wołoszyn, B. J. Spisak. “Simulations of transport characteristics of core-shell nanowire transistors with electrostatic all-around gate”. *Information Technology and Computational Physics*. Ed. by P. Kulczycki, L. T. Kóczy, R. Mesiar, J. Kacprzyk. Vol. 462. Advances in Intelligent Systems and Computing. Cham: Springer International Publishing, 2017, 233

My contribution to this publication was to take part in planning of the calculations, discussion of the results and preparation of the manuscript. I estimate my contribution to be 25%.

2. B. J. Spisak, M. Wołoszyn, P. Wójcik, G. J. Morgan. “Wigner distribution function description of a multilayered nanostructure with magnetic impurities”. *J. Phys.: Conf. Ser.* **193** (2009), 012130

My contribution to this publication was to participate in conceptual works, to write the computer programs used in all the calculations, and to execute them. I took part in discussion of the results, and in preparation of the manuscript. I estimate my contribution to be 45%.

3. M. Wołoszyn, B. J. Spisak. “Effect of structural disorder on the electronic density of states in one-dimensional chain of atoms”. *Computational Science - ICCS 2004: 4th International Conference, Kraków, Poland, June 6-9, 2004, Proceedings, Part II*. ed. by M. Bubak, G. D. van Albada, P. M. A. Sloot, J. Dongarra. Vol. 3037. Lecture Notes in Computer Science. Berlin, Heidelberg: Springer Berlin Heidelberg, 2004, 630

My contribution to this publication was to participate in planning of the research. I prepared the computer program and performed all calculations. I also took part in discussion of the results, and I wrote the manuscript of publication. I estimate my contribution to be 75%.

4. M. Wołoszyn, A. Z. Maksymowicz. “Coherent potential approximation technique in a simple example of resistivity calculations for binary alloys”. *TASK Quarterly : Scientific Bulletin of Academic Computer Centre in Gdansk* **85** (2002), 1–7

My contribution to this publication was to participate in planning of the research. I prepared the computer program for numerical calculations, executed them, and performed the analytical calculations. I also took part in discussion of the results, and preparation of the manuscript. I estimate my contribution to be 70%.

## D) Joint publications, collections catalogued, databases prepared, professional assessments

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## E) Impact factor of all publications

The total impact factor of all publications listed in Appendix A: 55.42 (for works published in 2017, the impact factor for year 2016 was used as the newest available).

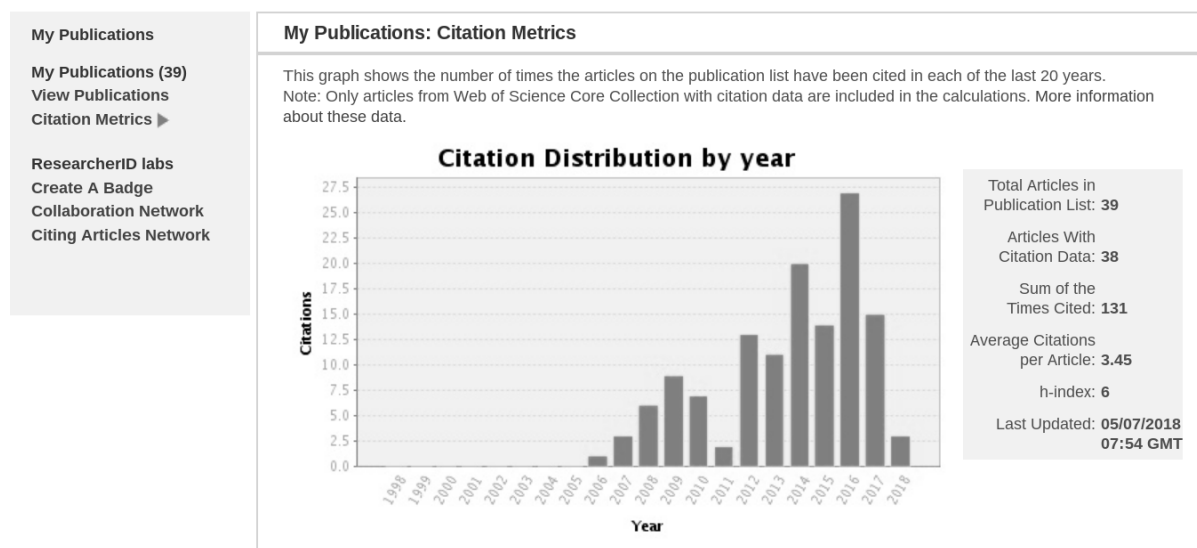
## F) The total number of citations according to Web of Science

The total number of citations to all publications is 131, and 74 without self-citations.

## G) Hirsch index according to Web of Science

$h = 6$ .

<b>Woloszyn, Maciej</b> <a href="#">Get A Badge</a> <a href="#">ResearcherID Labs</a>	
ResearcherID: C-8728-2011 URL: <a href="http://www.researcherid.com/rid/C-8728-2011">http://www.researcherid.com/rid/C-8728-2011</a> Subject: Physics ORCID: <a href="http://orcid.org/0000-0001-9896-1018">http://orcid.org/0000-0001-9896-1018</a>	My Institutions (more details) Primary Institution: AGH University of Science and Technology Sub-org/Dept: Role: Researcher (Academic)



## H) Leadership in international or national research projects or participation in such projects

- Participation in the project *Computer simulations of spin-dependent electronic transport in semiconductor quantum wires* as one of the principal investigators in the National Science Centre grant 2011/03/B/ST3/00240 (2012–2015).
- Participation in the project *Krakow Interdisciplinary PhD-Project in Nanoscience and Advanced Nanostructures* funded by Foundation for Polish Science within the International PhD Projects (MPD) from the Structural Funds (Operational Programme Innovative Economy), as a co-researcher of the research task *Modelling of quantum transport in semiconductor devices* (2009–2011).

## I) International and national awards for academic or artistic work

- Awards of the Rector of the Academy of Science and Technology for scientific achievements of the 2nd degree in years 2007, 2008, 2010, 2013.
- Awards of the Rector of the Academy of Science and Technology for scientific achievements of the 3rd degree in years 2008, 2014, 2015.

## J) Talks and lectures at scientific conferences

I presented the following talks at scientific conferences:

- *Transport properties of quasiperiodic systems*, 2nd International Wigner Workshop, Windermere, Great Britain, June 2017.
- *Application of the Wigner function to analysis of the transport properties of quasi-periodic systems*, XXI Symposium on Statistical Physics, Poznań, Poland, December 2016.
- *Transport of electrons in quasiperiodic multibarrier semiconductor nanowires*, Congress on Information Technology, Computational and Experimental Physics (CITCEP 2015), Kraków, Poland, December 2015.
- *Collective behaviour in clustered social networks*, 71st Annual Meeting of the Deutsche Physikalische Gesellschaft (DPG 2007), Regensburg, Germany, March 2007.

I am also the co-author of 10 other oral presentations at scientific conferences, listed in detail in Appendix C.

## 2.3. Achievements in teaching and popularization of science, research co-operation

### A) Participation in European programmes and other international or national programmes

- COST (European Cooperation in Science and Technology) Programme by European Science Foundation, grant for Short Term Scientific Mission within P10 Action (Topic: Interdisciplinary Monte Carlo simulations).

### B) Active participation in international or national academic conferences

Besides the oral presentations listed in 2.2J), I presented the following posters during the scientific conferences:

- *Phase-space dynamics of charge carriers in aperiodic potentials*, MECO43: 43rd Conference of the Middle European Cooperation in Statistical Physics, Kraków, Poland, May 2018.
- *Spin conductance of nanowires with double coupled quantum dots*, 44-th Jaszowiec International School and Conference on the Physics of Semiconductors, Wisła, Poland, June 2015.
- *Large magnetoresistance effect in cylindrical semiconductor nanowires with constriction*, The European Conference Physics Of Magnetism PM14, Poznań, Poland, June 2014.
- *Influence of dephasing time and geometrical parameters on the quantum corrections to the conductivity of cylindrical nanowire*, 42nd Jaszowiec International School and Conference on the Physics of Semiconductors, Wisła, Poland, June 2013.



- *Effect of localized magnetic moments configurations on the dynamics of electron wave packet – phase-space approach*, International Conference on Superlattices, Nanostructures and Nanodevices, Dresden, Germany, July 2012.
- *Localisation in semiconductor Fibonacci superlattice*, 5th Workshop on Quantum Chaos and Localisation Phenomena, Warszawa, Poland, May 2011.
- *Wigner distribution function description of a multilayered nanostructure with magnetic impurities*, 16th International Conference on Electron Dynamics In Semiconductors Optoelectronics and Nanostructures EDISON16, Montpellier, France, August 2009.
- *The Wigner function approach to spin-dependent electronic transport in presence of magnetic impurities*, Fifth International School and Conference on Spintronics and Quantum Information Technology SPINTECH5, Kraków, Poland, July 2009.
- *Computer simulation of the spin-polarised transport through a nanodevice*, Summer School Nanomagnetism and Spintronics, Praha, Czech Republic, September 2008.
- *Effect of magnetic dopants on transport properties of trilayer nanostructure*, SPINSWITCH Workshop – Spin Momentum Transfer, Kraków, Poland September 2008.
- *Influence of the electric field on the localisation in aperiodic quantum wires*, Conference on Computational Physics CCP2007, Brussels, Belgium, September 2007.
- *One-dimensional aperiodic systems in phase space*, XIX Marian Smoluchowski Symposium on Statistical Physics, Kraków, Poland, May 2006.
- *On the localization of electrons in disordered molecular wires*, Conference on New Concepts and Materials for Molecular Electronics and Nanotechnology CMME04, Puszczykowo, Poland, September 2004.
- *Effect of structural disorder on the electronic density of states in one-dimensional chain of atoms*, 4th International Conference on Computational Science ICCS2004, Kraków, Poland, June 2004.

I am also the co-author of 27 other poster presentations, listed in detail in Appendix C together with references to the publications related to the conference presentations.

### **C) Participation in organizing committees of international and national scientific conferences**

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### **D) Prizes and awards other than those indicated in 2.2I)**

—

### **E) Participation in consortiums and research networks**

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### **F) Management of scientific research and development projects performed in collaboration with national and international partners from science and industry, other than those indicated in 2.2H) above**

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## **G) Participation in editorial boards and other editorial activities**

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## **H) Membership in international or national organizations and scientific societies**

- Member of Polish Physical Society.

## **I) Achievements in teaching and popularization of science**

- Teaching activities in the years 2005–2018:
  - *Physics I* and *Physics II* – lectures, tutorial classes and laboratories for students of *Mechatronic Engineering with English as instruction language* at Faculty of Mechanical Engineering and Robotics, AGH University of Science and Technology (according to own syllabus),
  - *Object Oriented Programming I* and *Object Oriented Programming II* – lectures and laboratory classes at Faculty of Physics and Applied Computer Science (WFiIS), AGH University of Science and Technology (according to own syllabus),
  - *Graphical User Interface Programming* – lectures and laboratory classes at WFiIS AGH (according to own syllabus),
  - *Mathematical Methods of Physics* – seminars for PhD students at WFiIS AGH,
  - *C++ Language* – laboratory classes at WFiIS AGH,
  - *Procedural Programming* – laboratory classes at WFiIS AGH,
  - *Numerical Methods for Engineers* – laboratory classes at WFiIS AGH,
  - *Computer Numerical Simulations* – laboratory classes at WFiIS AGH,
  - *Fundamentals of Computer Science* – laboratory classes at WFiIS AGH,
  - *Unix System* – laboratory classes at WFiIS AGH.
- In order to prepare courses related to current IT techniques and modern programming languages, I have completed training organized by IBM and Microsoft.
- On the basis of student surveys in 2014 and 2016, I was placed on the list of the 10 best-rated academic teachers of WFiIS AGH which was prepared in years 2014–2016 (in 2015 I was not included because of the insufficient number of surveys carried out).
- Member of the organizing committee of the 6th and 7th edition of the *National Competition for the Physics Demonstration Experiments* organized by the Polish Physical Society (Kraków, 2006 and 2008).

## **J) Scientific assistance to students as scientific supervisor**

- Supervisor of 15 MSc theses at Faculty of Physics and Applied Computer Science (WFiIS), AGH University of Science and Technology.
- Supervisor of 27 BSc theses at WFiIS, AGH.
- Reviewer of 38 MSc theses.
- Reviewer of 52 BSc theses.
- Supervisor of the individual course of study of MSc student Mateusz Biliński at WFiIS, AGH.

### **K) Scientific assistance and co-supervision to PhD students**

- Co-supervision of PhD student Tomasz Palutkiewicz (since October 2015, in progress). Thesis title: *Computer simulations of electric charge transport in semiconductor core-shell nanowires*, Faculty of Physics and Applied Computer Science, AGH University of Science and Technology.

### **L) Internships in foreign research or academic centres**

- Department of Physics, University of Liege, Belgium (17/11/2006 to 27/11/2006, host: Prof. Marcel Ausloos)
- Institute for Theoretical Physics, University of Regensburg, Germany (19/04/2015 to 25/04/2015, host: Prof. Jaroslav Fabian)

### **M) Evaluations performed or other scientific studies made to order**

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### **N) Participation in expert and competition teams**

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### **O) Reviews of international and national research projects**

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### **P) Reviews of publications in international and national journals**

- Journal of Non-Crystalline Solids (3 reviews).
- Solid State Communications (2 reviews).
- Journal of Physics D: Applied Physics (1 review).
- Central European Journal of Physics (1 review).
- Physics Letters A (1 review).

### **Q) Activities other than those indicated in 2.3 A) – 2.3 P)**

- Member of commission supervising BSc theses of the Applied Computer Science students at Faculty of Physics and Applied Computer Science (WFiIS), AGH University of Science and Technology (since 2014).
- Member of the Faculty Team for Quality of Education supervising preparation of syllabuses with regard to National Qualifications Framework, WFiIS AGH (2011–2012).
- Member of the examination board for admissions to the second degree of studies, WFiIS AGH (2007–2009).
- Member of the commission conducting final exams for BSc degree, WFiIS AGH (since 2013).





## A. Scientific publications in journals covered by the Journal Citation Reports (JCR) database

Complete list of all publications, including the publications which are the basis of the achievement.

- [A1] M. Wołoszyn, B. J. Spisak. “Dissipative transport of thermalized electrons through a nanodevice”. *Phys. Rev. B* **96** (2017), 075440.
- [A2] M. Wołoszyn, B. J. Spisak. “Stark resonances induced by the exchange–correlation potential in piezoelectric nanowires”. *Phys. Status Solidi RRL* **11** (2017), 1700248.
- [A3] U. Kaczor, M. Wołoszyn, B. J. Spisak. “Phase-space approach to the position-momentum correlations of the conduction electron states in a double-barrier resonant nanosystem”. *Acta Phys. Pol. A* **132** (2017), 106.
- [A4] M. Wołoszyn, B. J. Spisak, P. Wójcik, J. Adamowski. “Transition from positive to negative magnetoresistance induced by a constriction in semiconductor nanowire”. *Physica E* **83** (2016), 127.
- [A5] M. Wołoszyn, B. J. Spisak, P. Wójcik, J. Adamowski. “Spin conductance of nanowires with double coupled quantum dots”. *Acta Phys. Pol. A* **129** (2016), A–114.
- [A6] T. Palutkiewicz, M. Wołoszyn, P. Wójcik, B. J. Spisak. “Transport characteristics of gated core-multishell nanowires: self-consistent approach”. *Acta Phys. Pol. A* **130** (2016), 1190.
- [A7] T. Palutkiewicz, M. Wołoszyn, P. Wójcik, J. Adamowski, B. J. Spisak. “Influence of geometrical parameters on the transport characteristics of gated core-multishell nanowires”. *Acta Phys. Pol. A* **129** (2016), A–111.
- [A8] U. Kaczor, B. Klimas, D. Szydłowski, M. Wołoszyn, B. J. Spisak. “Phase-space description of the coherent state dynamics in a small one-dimensional system”. *Open Phys.* **14** (2016), 354.
- [A9] B. J. Spisak, M. Wołoszyn. “Quantum kinetic theory of the  $2k_F$  scattering mechanism for three-dimensional structurally disordered systems in the Ioffe-Regel limit”. *Acta Phys. Pol. A* **128** (2015), 213.
- [A10] B. J. Spisak, M. Wołoszyn, D. Szydłowski. “Dynamical localisation of conduction electrons in one-dimensional disordered systems”. *J. Comput. Electron.* **14** (2015), 916.
- [A11] P. Wójcik, J. Adamowski, M. Wołoszyn, B. J. Spisak. “Spin splitting generated in a Y-shaped semiconductor nanostructure with a quantum point contact”. *J. Appl. Phys.* **118**, 014302 (2015), 014302.
- [A12] P. Wójcik, J. Adamowski, M. Wołoszyn, B. J. Spisak. “Resonant Landau–Zener transitions in a helical magnetic field”. *Semicond. Sci. Technol.* **30** (2015), 065007.
- [A13] M. Wołoszyn, B. J. Spisak, J. Adamowski, P. Wójcik. “Magnetoresistance anomalies resulting from Stark resonances in semiconductor nanowires with a constriction”. *J. Phys. Condens. Matter* **26** (2014), 325301.

- [A14] P. Wójcik, J. Adamowski, B. J. Spisak, M. Wołoszyn. “Spin transistor operation driven by the Rashba spin-orbit coupling in the gated nanowire”. *J. Appl. Phys.* **115**, 104310 (2014), 104310.
- [A15] P. Wójcik, J. Adamowski, M. Wołoszyn, B. J. Spisak. “All-electrical manipulation of electron spin in a semiconductor nanotube”. *Physica E* **59** (2014), 19.
- [A16] M. Wołoszyn, J. Adamowski, P. Wójcik, B. J. Spisak. “Periodicity of resonant tunneling current induced by the Stark resonances in semiconductor nanowire”. *J. Appl. Phys.* **114** (2013), 164301.
- [A17] B. J. Spisak, M. Wołoszyn, P. Wójcik. “Influence of dephasing and geometrical parameters on quantum correction to dc conductance of cylindrical nanowires”. *Acta Phys. Pol. A* **124** (2013), 838.
- [A18] D. Szydłowski, M. Wołoszyn, B. J. Spisak. “Phase-space description of wave packet approach to electronic transport in nanoscale systems”. *Semicond. Sci. Technol.* **28** (2013), 105022.
- [A19] P. Wójcik, J. Adamowski, M. Wołoszyn, B. J. Spisak. “Spin filter effect at room temperature in GaN/GaMnN ferromagnetic resonant tunnelling diode”. *Appl. Phys. Lett.* **102**, 242411 (2013), 242411.
- [A20] M. Wołoszyn, B. J. Spisak. “Multifractal analysis of the electronic states in the Fibonacci superlattice under weak electric fields”. *Eur. Phys. J. B* **85** (2012), 10.
- [A21] P. Wójcik, J. Adamowski, M. Wołoszyn, B. J. Spisak. “Intrinsic oscillations of spin current polarization in a paramagnetic resonant tunneling diode”. *Phys. Rev. B* **86** (2012), 165318.
- [A22] P. Wójcik, B. J. Spisak, M. Wołoszyn, J. Adamowski. “Hysteresis loops of spin-dependent electronic current in a paramagnetic resonant tunnelling diode”. *Semicond. Sci. Technol.* **27** (2012), 115004.
- [A23] P. Wójcik, B. J. Spisak, M. Wołoszyn, J. Adamowski. “Tuning of terahertz intrinsic oscillations in asymmetric triple-barrier resonant tunneling diodes”. *J. Appl. Phys.* **111**, 124310 (2012), 124310.
- [A24] P. Wójcik, B. J. Spisak, M. Wołoszyn, J. Adamowski. “Simulation of spin-dependent electronic transport through resonant tunnelling diode with paramagnetic quantum well”. *Acta Phys. Pol. A* **119** (2011), 648.
- [A25] P. Wójcik, A. Naylor, M. Wołoszyn, B. Hickey, B. J. Spisak, J. Adamowski. “Influence of barrier width on spin-polarisation measured by point contact Andreev reflection”. *J. Supercond. Nov. Magn.* **24** (2011), 939.
- [A26] P. Wójcik, B. J. Spisak, M. Wołoszyn, J. Adamowski. “Intrinsic current oscillations in an asymmetric triple-barrier resonant tunnelling diode”. *Semicond. Sci. Technol.* **25** (2010), 125012.
- [A27] P. Wójcik, B. J. Spisak, M. Wołoszyn, J. Adamowski. “Self-consistent Wigner distribution function study of gate-voltage controlled triple-barrier resonant tunnelling diode”. *Semicond. Sci. Technol.* **24** (2009), 095012.
- [A28] B. J. Spisak, M. Wołoszyn. “Nonclassical properties of electronic states of aperiodic chains in a homogeneous electric field”. *Phys. Rev. B* **80** (2009), 035127.
- [A29] B. J. Spisak, M. Wołoszyn, A. Paja. “Spin-dependent transport through metallic system with magnetic impurities”. *Acta Phys. Pol. A* **115** (2009), 266.
- [A30] P. Wójcik, B. J. Spisak, M. Wołoszyn, J. Adamowski. “Application of non-classical distribution function to the transport properties of semiconductor nanodevices”. *Acta Phys. Pol. A* **114** (2008), 1431.

- [A31] M. Wołoszyn, D. Stauffer, K. Kułakowski. “Order-disorder phase transition in a cliquy social network”. *Eur. Phys. J. B* **57** (2007), 331.
- [A32] B. J. Spisak, M. Wołoszyn. “One-dimensional aperiodic systems in phase space”. *Acta Phys. Pol. B* **38** (2007), 1951.
- [A33] M. Wołoszyn, D. Stauffer, K. Kułakowski. “Phase transitions in Nowak-Sznajd opinion dynamics”. *Physica A* **378** (2007), 453.
- [A34] A. Z. Maksymowicz, M. Wołoszyn. “Density of states in structurally disordered 1D chains of atoms”. *J. Non-Cryst. Solids* **352** (2006), 4200.
- [A35] M. Wołoszyn, B. J. Spisak, A. Z. Maksymowicz. “Phase space description of localization in disordered one-dimensional systems”. *Acta Phys. Pol. A* **110** (2006), 523.
- [A36] M. Wołoszyn, B. J. Spisak. “On the localization of electrons in disordered molecular wires”. *Materials Science (Poland)* **22** (2004), 545.

## B. Scientific publications in journals not covered by the Journal Citation Reports (JCR) database

- [B1] T. Palutkiewicz, M. Wołoszyn, B. J. Spisak. “Simulations of transport characteristics of core-shell nanowire transistors with electrostatic all-around gate”. *Information Technology and Computational Physics*. Ed. by P. Kulczycki, L. T. Kóczy, R. Mesiar, J. Kacprzyk. Vol. 462. Advances in Intelligent Systems and Computing. Cham: Springer International Publishing, 2017, 233.
- [B2] B. J. Spisak, M. Wołoszyn, P. Wójcik, G. J. Morgan. “Wigner distribution function description of a multilayered nanostructure with magnetic impurities”. *J. Phys.: Conf. Ser.* **193** (2009), 012130.
- [B3] M. Wołoszyn, B. J. Spisak. “Effect of structural disorder on the electronic density of states in one-dimensional chain of atoms”. *Computational Science - ICCS 2004: 4th International Conference, Kraków, Poland, June 6-9, 2004, Proceedings, Part II*. Ed. by M. Bubak, G. D. van Albada, P. M. A. Sloot, J. Dongarra. Vol. 3037. Lecture Notes in Computer Science. Berlin, Heidelberg: Springer Berlin Heidelberg, 2004, 630.
- [B4] M. Wołoszyn, A. Z. Maksymowicz. “Coherent potential approximation technique in a simple example of resistivity calculations for binary alloys”. *TASK Quarterly : Scientific Bulletin of Academic Computer Centre in Gdansk* **85** (2002), 1–7.



## C. Conference contributions

### 1. Oral presentations

- [C1.1] M. Wołoszyn, B. J. Spisak. “Transport properties of quasiperiodic systems”. *2nd International Wigner Workshop*. Windermere (GB). 2017.
- [C1.2] B. J. Spisak, M. Wołoszyn. “Non-classical properties of electronic states. Influence of the scattering mechanisms”. *2nd International Wigner Workshop*. Windermere (GB). 2017.
- [C1.3] J. Adamowski, P. Wójcik, B. J. Spisak, M. Wołoszyn. “Nanowire-based spintronic analogs of optical devices”. *BIT’s 2nd Annual World Congress of Smart Materials*. Singapore. 2016.
- [C1.4] M. Wołoszyn. “Zastosowanie funkcji Wignera do analizy własności transportowych układów kwaziperiodycznych”. *XXI Minisymposium Fizyki Statystycznej*. Poznań (PL). 2016.
- [C1.5] T. Palutkiewicz, M. Wołoszyn, B. J. Spisak. “Simulations of transport characteristics of core-shell nanowire transistors with electrostatic all-around gate”. *Congress on Information Technology, Computational and Experimental Physics (CITCEP 2015)*. Kraków (PL). 2015. [B1].
- [C1.6] U. Kaczor, B. Klimas, D. Szydłowski, M. Wołoszyn, B. J. Spisak. “Phase-space description of the coherent state dynamics in one-dimensional small system”. *Congress on Information Technology, Computational and Experimental Physics (CITCEP 2015)*. Kraków (PL). 2015. [A8].
- [C1.7] M. Wołoszyn, B. J. Spisak. “Transport of electrons in quasiperiodic multibarrier semiconductor nanowires”. *Congress on Information Technology, Computational and Experimental Physics (CITCEP 2015)*. Kraków (PL). 2015.
- [C1.8] B. J. Spisak, M. Wołoszyn. “Wigner representation of dynamics and dephasing of electrons in disordered systems”. *International Symposium on Advanced Nanodevices and Nanotechnology (ISANN 2015)*. Waikoloa, Hawaii (USA). 2015.
- [C1.9] B. J. Spisak, M. Wołoszyn. “Wigner representation of dynamics and dephasing of electrons in disordered systems”. *International Wigner Workshop*. Waikoloa, Hawaii (USA). 2015.
- [C1.10] J. Adamowski, P. Wójcik, B. J. Spisak, M. Wołoszyn. “Physics of nanowire spintronic devices”. *From Spins to Cooper Pairs: New Physics of the Spins (StoCP-2014)*. Zakopane (PL). 2014.
- [C1.11] P. Wójcik, J. Adamowski, B. J. Spisak, M. Wołoszyn. “Spin transistor action driven by the helical magnetic field”. *From Spins to Cooper Pairs: New Physics of the Spins (StoCP-2014)*. Zakopane (PL). 2014.
- [C1.12] J. Adamowski, P. Wójcik, B. J. Spisak, M. Wołoszyn. “Spin-polarized electron current modification in gated semiconductor nanowires”. *Energy-Materials-Nanotechnology Fall Meeting*. Orlando (US). 2013.
- [C1.13] M. Wołoszyn, D. Stauffer, K. Kułakowski. “Collective behaviour in clustered social networks”. *71st Annual Meeting of the Deutsche Physikalische Gesellschaft DPG2007*. Regensburg (DE). 2007.

- [C1.14] A. Z. Maksymowicz, M. Wołoszyn. “Density of states in structurally disordered 1D chains of atoms”. *3rd International Conference Physics of Disordered Systems PDS05*. Gdańsk-Sobieszewo (PL). 2005. [A34].

## 2. Poster sessions

- [C2.1] M. Wołoszyn, B. J. Spisak. “Phase-space dynamics of charge carriers in aperiodic potentials”. *MECO43: 43rd Conference of the Middle European Cooperation in Statistical Physics*. Kraków (PL). 2018.
- [C2.2] D. Kołaczek, M. Wołoszyn, B. J. Spisak. “Time evolution of the Wigner function for the generalized Schrödinger cat state”. *MECO43: 43rd Conference of the Middle European Cooperation in Statistical Physics*. Kraków (PL). 2018.
- [C2.3] B. J. Spisak, M. Wołoszyn. “Phase-space dynamics of quantum systems with dissipation”. *Frontiers of Quantum and Mesoscopic Thermodynamics*. Praha (CZ). 2017.
- [C2.4] B. J. Spisak, M. Wołoszyn, U. Kaczor. “Phase-space approach to position-momentum correlations induced by the quantum interference phenomena in resonant-tunneling nanosystems”. *The Twelfth International School on Theoretical Physics Symmetry and Structural Properties of Condensed Matter*. Rzeszów (PL). 2016. [A3].
- [C2.5] T. Palutkiewicz, M. Wołoszyn, P. Wójcik, B. J. Spisak. “Transport characteristics of gated core-multishell nanowires: self-consistent approach”. *45th "Jaszowiec" International School and Conference on the Physics of Semiconductors*. Szczyrk (PL). 2016. [A6].
- [C2.6] B. J. Spisak, M. Wołoszyn. “Dynamical localization of the wave packet in disordered environment: phase-space approach”. *7th Workshop on Quantum Chaos and Localisation Phenomena*. Warszawa (PL). 2015.
- [C2.7] P. Wójcik, J. Adamowski, M. Wołoszyn, B. J. Spisak. “Effect of nonadiabaticity on spin transitions in helical magnetic field”. *SPINTECH VIII International School and Conference*. Basel (CH). 2015.
- [C2.8] B. J. Spisak, M. Wołoszyn. “Dynamics of the quantum state in small systems under influence of statistical field. Phase-space approach”. *Frontiers of Quantum and Mesoscopic Thermodynamics*. Praha (CZ). 2015.
- [C2.9] M. Wołoszyn, J. Adamowski, P. Wójcik, B. J. Spisak. “Spin conductance of nanowires with double coupled quantum dots”. *44-th Jaszowiec International School and Conference on the Physics of Semiconductors*. Wisła (PL). 2015. [A5].
- [C2.10] T. Palutkiewicz, M. Wołoszyn, P. Wójcik, J. Adamowski, B. J. Spisak. “Influence of geometrical parameters on the transport characteristics of gated core-multishell nanowires”. *44-th Jaszowiec International School and Conference on the Physics of Semiconductors*. Wisła (PL). 2015. [A7].
- [C2.11] P. Wójcik, J. Adamowski, M. Wołoszyn, B. J. Spisak. “Generating and detecting the spin current in Y-shaped semiconductor nanowire with quantum point contact”. *nanoPT Nanoscience and Nanotechnology International Conference*. Porto (PT). 2015.
- [C2.12] M. Wołoszyn, B. J. Spisak, P. Wójcik, J. Adamowski. “Spin-dependent magnetotransport properties of double-gate semiconductor nanowires”. *Theory, Modelling and Computational Methods for Semiconductors*. Granada (ES). 2015.
- [C2.13] B. J. Spisak, M. Wołoszyn, P. Wójcik, J. Adamowski. “Spin-dependent magnetotransport through quantum point contact in semiconductor nanowires”. *Theory, Modelling and Computational Methods for Semiconductors*. Granada (ES). 2015.

- [C2.14] B. J. Spisak, M. Wołoszyn. “Dynamical localization of quantum states in the one-dimensional disordered environment. View from the phase-space perspective”. *27th Marian Smoluchowski Symposium on Statistical Physics*. Zakopane (PL). 2014.
- [C2.15] B. J. Spisak, M. Wołoszyn. “Influence of dephasing processes on the  $2k_F$  scattering mechanism of conduction electrons in three-dimensional structurally disordered systems”. *The 11th International School on Theoretical Physics: Symmetry and Structural Properties of Condensed Matter*. Rzeszów (PL). 2014. [A9].
- [C2.16] B. J. Spisak, M. Wołoszyn, J. Adamowski, P. Wójcik. “Spin-dependent magnetotransport in semiconductor nanowires”. *The European Conference Physics Of Magnetism PM14*. Poznań (PL). 2014.
- [C2.17] M. Wołoszyn, B. J. Spisak, P. Wójcik, J. Adamowski. “Large magnetoresistance effect in cylindrical semiconductor nanowires with constriction”. *The European Conference Physics Of Magnetism PM14*. Poznań (PL). 2014.
- [C2.18] M. Wołoszyn, B. J. Spisak, P. Wójcik, J. Adamowski. “Effect of a double constriction on the magnetotransport properties of semiconductor nanowires”. *43rd Jaszowiec International School and Conference on the Physics of Semiconductors*. Wisła (PL). 2014.
- [C2.19] P. Wójcik, J. Adamowski, B. J. Spisak, M. Wołoszyn. “Modification of electron spin induced by the Rashba spin-orbit interaction in a semiconductor nanotube”. *5th International Conference on One-dimensional Nanomaterials*. Annecy (FR). 2013.
- [C2.20] B. J. Spisak, P. Wójcik, M. Wołoszyn, J. Adamowski. “Computer simulations of spin transistor operation in InAs nanowire”. *5th International Conference on One-dimensional Nanomaterials*. Annecy (FR). 2013.
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