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Report on the doctoral dissertation of Mr Michał Nowak: "Electronic structure of artificial atoms and molecules: spin-orbit coupling effects"

The thesis consists of a collection of eight papers [A.1 – A.8] and a manuscript [M.1] supplied with a short introduction and summary of the articles. All the papers have been published in one of highly ranked scientific journals – the Physical Review B. Mr Nowak is the first author of all the publications, which together with declarations of co-authorship, signed by Prof. Francois Peeters, Prof. Bart Partoens, Prof. Bartłomiej Szafran and Mr Wojciech Pasek, makes his contribution to above mentioned papers significant and predominant.

Recently a significant progress has been made in fabrication of single and coupled quantum dots, often called artificial atoms and molecules due to their discrete electron energy spectra. This opened a route to study quantum phenomena at the atomic scale and paved the way to design and produce more sophisticate systems with application in nanoelectronics and quantum computing. In particular, the ability to control spin of a single electron is highly demanded, as the electron spin in a quantum dot has been proposed to play a role of a quantum information bit (qubit). Unfortunately, the usual way of controlling the electron spin by external magnetic field turns out to be inefficient. Thus other alternatives have been considered. One of possibilities is to control the electron spin electrically utilizing the spin-orbit coupling. There are two possible realizations of the spin-orbit interaction: due to the lack of an inversion symmetry of the structure (Rashba) and of the crystal lattice (Dresselhaus effect).

The research presented in the thesis concerns theoretical description of spin-orbit coupling effects in nanoscale devices – quantum dot and quantum ring systems. A particular emphasis is put on spin control by the orbital degrees of freedom of electrons confined in quantum dots. The present work refers also to some recent experiments on self-assembled quantum dots and gate-controlled nanowires. In particular, the transport spectroscopy of a single self-organized quantum dot and the electric dipole spin resonance spectroscopy measurements have been discussed. In his study the author uses mainly configuration interaction approach to solve an eigenproblem of a given Hamiltonian, which is a powerful technique to study electronic properties of nanoscale systems.

In the following I will summarize the most interesting results obtained by Mr Nowak during his Ph.D. studies, presented and discussed in papers [A.1 – A.8] and in manuscript [M.1].

Paper [A.1] discusses the problem of spin-orbit interaction in few-electron quasi-two-dimensional double quantum dots. A particular emphasis is put on the mixing of bonding and antibonding electron orbitals induced by spin-orbit interaction and its consequences for optical absorption spectra. To tackle the problem, the authors developed a technique featuring the spin-dependent single electron states calculated in Gaussian function basis defined on a square grid. This approach captures both the Rashba and Dresellhaus spin-orbit couplings in systems without any symmetry. The calculation shows that the spin-orbit interaction opens avoided crossing between the states of opposite spin orientation and spatial parity in the case of odd number of electrons (one and three studied here). On the other hand, for two electrons, this manifests itself in low energy optical transitions, which were forbidden in the system without spin-orbit coupling.

A starting point of investigations presented in work [A.2] was an ongoing discussion on spin exchange between two electrons in double quantum dot systems. In their study, the authors focus on a spin dynamics of a double quantum dot in zero magnetic field, in particular, in the presence of spin-orbit and electron-electron interactions. The time-dependent simulations show that four different processes contribute to the spin swap for two-electron double quantum dot. Those include: a direct tunneling of electrons between the dots, the spin tunneling, the spin precession due to the spin-orbit interaction, and a generation of opposite spin components in the direction of the effective spin-orbit magnetic fields. While the charge transport between the dots can be suppressed effectively by the Coulomb repulsion, the spin tunneling and spin precession are still allowed. The Coulomb interaction is responsible also for the last process listed above, which has its origin in a collective motion of the electrons within the inner degrees of freedom, and is necessary to maintain a constant electron-electron distance. Furthermore, the spin swap is substantially modified by the double dot orientation with respect to the crystal lattice, and can be isotropic for a proper orientation of the dots and equal Rashba and Dresselhaus constants.

The influence of a spatial orientation of coupled quantum dots on the energy splitting between the states of opposite spin in the presence of spin-orbit interactions was the main subject of the study presented in paper [A.3]. It was shown that the width of the avoided crossings can be tuned to a large extent by the anisotropy of spin-orbit coupling, and thus by orientation of the quantum dot with respect to the crystal lattice. Both Rashba and Dresselhaus interactions with comparable magnitudes of the coupling constants must operate at the same time. The avoided crossing changes come from an anisotropic Zeeman interaction, which polarizes the spins in the direction of the external magnetic field and suppresses the spin-orbit effects. The dot orientation affects also the effective Landé g factor.

In publication [A.4] one and two electrons confined in two-dimensional quantum ring in the presence of spin orbit interactions have been considered. It is demonstrated that the charge density deviates from the circular symmetry defined by the confinement potential provided the Zeeman effect is present or Rashba and Dresselhous coupling constants are equal to each other. In the case of two electrons the deformation of charge density can be increased by the Coulomb interaction. It was also found that similar results can be obtained in the case of an elliptical deformation of the quantum ring confinement potential. All the results obtained in paper [A.4] were confronted with the lowest-radial state approximation, i.e. one-dimensional ring model. It was shown that the lowest-radial state approximation leads to some artifacts, in particular when both Rashba and Dresselhous interactions are present.

A quantum dot in the geometry of a ring is also discussed in work [A.5]. In this case the electron transport through the quantum ring in the presence of Rashba spin-orbit coupling has been investigated within linear response theory. Similar as in paper [A.4] two-dimensional channels in the

ring have been taken into account. The main results concern the appearance of sharp Fano resonances around Aharonov-Casher oscillation maxima in the conductance. It was shown that these resonances appear as a consequence of the coupling of current carrying states from the leads with the states localized in the ring, which is possible owing to the spin-orbit induced parity breaking of the ring states. The Fano resonances become broadened when the spin-orbit interaction is detuned from the Aharonov-Casher maxima. As a result the spin transport strongly depends on the Fermi energy. It is worthwhile to note, that in the case of the one-dimensional ring this effect is absent.

In paper [A.6] the energy spectrum of single and two-electron spin-orbit-coupled three-dimensional quantum dots is studied in the presence of an external magnetic field. This paper refers to the transport spectroscopy experiment on a single gated self-assembled quantum dot [S. Takahashi *et al.*, Phys. Rev. Lett. **104**, 246801 (2010)], in which broad anticrossings in the energy spectra and their dependence on the orientation of the external magnetic field have been observed. Present work is the first successful theoretical attempt to describe and understand the phenomena observed in the above-mentioned experiment. The experimentally determined anticrossing width dependence on the direction of the in-plane magnetic field turns out to be related to the individual spin-orbit couplings and the anisotropy of the confinement potential. Furthermore, the authors provide also analytic formula which allows to determine the relative strengths of the individual spin-orbit interactions from the experimental data.

A motivation to the study presented in work [A.7] comes from electric-dipole spin resonance experiments on gated nanowires, where fractional resonances and a splitting of the central line have been observed. The authors developed a computational scheme to simulate the spin rotations induced by an ac electric field in a two-electron double quantum dot. The calculation reveals that the spin exchange interaction leads to the splitting of the central resonance line accompanied by the fractional resonances. Both effects turn out to be induced by interdot tunnel coupling. Furthermore, the ac electric field generates residual harmonics of the driving frequency, which can be amplified when brought to the Rabi main transition frequency. It turns out that this mechanism is a common feature of the quantum dot systems subject to ac electric field.

Publication [A.8] deals with the anisotropy of spin polarization in a narrow nanowire quantum dot in the presence of spin-orbit interaction. The obtained results reveal a strong dependence of the spin polarization on the system geometry and on the external magnetic field orientation, with easy and hard axes observed. Interestingly, in the case of strong lateral confinement the electron spin can become well defined even in the presence of spin-orbit coupling. The authors study the nanowire quantum dot in one-dimensional limit analytically, and provide a formula for an effective Landé g factor which depends on the orientation of the external magnetic field. The present calculation reproduces well the experimentally determined magnetic-field-orientation dependence of the effective g factor and avoided crossing width.

In manuscript [M.1] the phonon mediated electron relaxation in nanowire quantum dots under ac electric field is discussed, in particular in the context of spin blockade lifting. Considering the dynamics of the system, the authors predicted that the spin blockade can be removed by phonon mediated relaxation. This can happen if the energy of initial state is close to the ground state energy. As a result only the spin triplet state with antiparallel orientation is blocked in a weak magnetic field. At higher magnetic field, when the spin triplet is the ground state the spin blockade is lifted owing to the opening of an additional channel associated with the spin rotation and charge redistribution. The obtained results are confronted with recent electric dipole spin resonance experiments.

To summarize, Mr Michał Nowak performed a deep theoretical analysis of spin-orbit effects in various realizations of quantum dot systems. He obtained many interesting and important results, solving the Schrödinger equation for different systems in its time-dependent or in time-independent form, according to the problem considered. It is clear that Mr Nowak mastered the advanced theoretical physics methods and their numerical implementations perfectly, as all the calculations were done by him. The present study features a great ingenuity, thoroughness and reliability, and substantially widens our understanding of physical phenomena at nanoscale. It is also important that much effort has been done to explain a number of experimental findings and to predict new effects, which can be verified by experiments. Such a tight interaction between theory and experiment is always advantageous.

In my opinion the thesis submitted by Mr Michał Nowak fully meets the requirements for the doctoral degree in physics and I recommend that the next steps of the procedure are initiated. Having considered the number and high scientific level of publications I think the dissertation should be given a distinction.

Mariusz Krawiec