Nanophysics Center, Reykjavik University
Annual Report 2017

Members of the group

The Nanophysics Center (Website nano.ru.is) had eleven members during 2016. Five members are faculty staff, Andrei Manolescu, Ágúst Valfells, Halldór Svavarsson, Sigurður Ingi Erlingsson, and Gunnar Þorgilsson. Gunnar moved from RU to ISOR, he is still a collaborator. Anna Sitek and Kristinn Torfason are postdoctoral researchers. Muhammad Taha Sultan and Miguel Urbaneja are PhD students, both in their second year. Hákon Örn Árnason is a Master student and Hákon Valur Haraldsson is a BS student who graduated at the end of 2017. Aitor Gonzalez is an MSc student who did his thesis within the Nanophysics Center as an exchange student from Lund University in Sweden.

Main research projects: participants, results, work in progress

Magnetoresistance oscillations in systems with spin-orbit coupling.
This is a collaboration between Sigurður I. Erlingsson and Prof. J. Carlos Egues at the University of Sao Paulo, Sao Carlos. The main result is an equation that describes beatings in the Shubnikov-de Haas oscillations in a 2D electron gas with both Rashba and Dresselhaus interaction. The central feature of the project is a new approximation scheme that works well for strong spin-orbit coupling and high Landau-level index. This year a new experiment was published with magnetoresistance resistance measurements with strong spin-orbit coupling and we had to improve our approximation method to be able to describe those measurements. The updated manuscript is in preparation with input from the experimental group of Prof. Dominik Zumbuhl at the University of Basel that does magnetoresistance measurements.

Topological insulators.
Sigurður Erlingsson has continued his work on magnetic impurities in topological insulators. The analytical work done by an undergraduate student last year served as a motivation to do numerical modeling on the effects of magnetic impurities. The goal of this project is to compare the results of the diagrammatic method with the numerics, and determine whether transport measurements (the conductance) will yield more information about the effects of the magnetic impurities than optical methods (the density of states). A manuscript is in preparation. This project involves Dr. Karel Vyborny from Institute of Physics in Prague and Simon Wozny from the University of Konstanz.
Simon Wozny visited Nanophysics Center for two weeks in April.

Electronic transport in open nanosystems in the presence of photons.
This work is on electronic states and transport in nanosystems coupled to cavity photons, described with the generalized non-Markovian master equation, with the participation of Andrei Manolescu and Anna Sitek, in collaboration with Viðar Guðmundsson and his group from University of Iceland. The funding was obtained by VG from the Icelandic Research Fund in 2016. The main results obtained in 2017 are the electroluminescence caused by the transport of electrons through two parallel quantum dots in an optical photon cavity, and the identification of the radiative and non-radiative transitions in the many-body system via the current correlations. Next steps will be to consider correlations of electrons via photons and phonons.

Optical properties of core-shell semiconductor nanowires.

This was the main activity of Anna Sitek, with the increasing contribution of Miguel Urbaneja, supervised by Andrei Manolescu. The many-body states of valence and conduction electrons in core-shell nanowires with polygonal cross section, with Coulomb interaction included, are obtained numerically. Kristinn Torfason helped with parallelizing the code and prepared a version for the GPU card, which considerably reduced the computational time. The main focus was on the behavior of the electronic states localized on the corners of the polygon and on the sides of the polygon, respectively. The results show that the optically active excitons are typically produced by the states with energy within the gap between the corner and side states, which are a result of many-body Coulomb interaction.

Electronic transport in core-shell semiconductor nanowires.
Miguel Urbaneja performed transport calculations in core-shell nanowires with polygonal geometry, in close collaboration with Anna Sitek, with computational help from Kristinn Torfason, and supervised by Andrei Manolescu. He implemented the Hartree-Fock approximation in the energy spectra and he obtained interesting exchange effects that can influence the conductance. He also calculated the conductance steps assuming ballistic transport, and also nonlinear I-V characteristics, and he started working on impurity effects. He also obtained the currents generated by an AC voltage acting on a prismatic nanowire and he calculated the electromagnetic field radiated by a core-shell antenna. Sigurður Erlingsson and Gunnar Þorgilsson performed calculations of the current generated in a cylindrical shell due to a temperature gradient, in the presence of a magnetic field perpendicular to the cylinder, and demonstrated that the current can change sign for a strong magnetic field such that the cyclotron and snaking orbits coexist. This phenomenon is expected to be robust to impurities, both in normal and in topological nanowires.

Majorana states in core-shell prismatic nanowires.
Andrei Manolescu and Anna Sitek, in collaboration with Llorens Serra and Javier Osca, from University of Balearic Islands, Mallorca, Tudor Stanescu from West Virginia University, and Vidar Gudmundsson from University of Iceland, showed that the low energy electronic states localized at the edges of a prismatic core-shell nanowire can generate multiple Majorana states. Depending on the thickness of the shell, the Majorana states can be isolated or can interact. In the latter case, the phase diagrams are specific to the nanowire geometry and symmetry.

Photovoltaic applications of Silicon nanowires.
The project is done in cooperation with the Nanophotonic Device group at University of Texas at Arlington (UTA). Halldór Svavarsson together with Master's student Hákon Örn Árnason made a new setup and started measurements of thermal conductivity of arrays of Silicon nanowires. Until the end of the year, the measurements were in the calibration stage. Almost a year ago, Hákon prepared flat p-n junctions by diffusion of antimony into silicon wafer for photovoltaic applications. At the present state, he has further managed to prepare functional photovoltaic device of SiNWs (SiNWs solar cell). A newly purchased solar-simulator was used to measure the open-circuit voltage and efficiency of the device. Hákon, together with PhD student Taha, designed and built an instrument for hydrogenation that was used to hydrogenate the SiNWs solar cell. A 40% increase in efficiency of the cell was observed by that. The funding of this project is provided by the Energy Fund of the National Power Company of Iceland (Landsvirkjun).

TiO_2 thin films with embedded GeSi nanoparticles.
This project started in 2016 and it is funded by Rannis with an M-ERA.NET collaboration with National Institute of Materials Physics from Romania. The PhD student Muhammad Taha Sultan, under the close supervision of Halldór Svavarsson, grew high quality TiO_2 layers with GeSi nanoparticles using Hi Power Impulse Magnetron Sputtering. The hydrogenation chamber (see text above), built for this project, was used to hydrogenate selected samples. A significant improvement in the light sensitivity of the samples

was observed. A manuscript on Photoconductivity of GeSi nanoparticles embedded in TiO_2 matrix is now in preparation.

SiO_2 thin films with embedded GeSi nanoparticles.
An exchange student Aitor Gonzalez, enrolled at Lund University in Sweden, was working on this topic, using similar approach as PhD student Taha (see above). Aitor spent roughly 6 months in Iceland working on this project under Halldór's supervision and with help from Taha. Aitor is supposed to defend his thesis at Lund in 15 January 2018.

Electronic properties of vacuum diodes.
Kristinn Torfason continued to improve the capabilities of the molecular dynamics code, adding the following features: calculate the emittance, velocity distribution, Shockley–Ramo current, inclusion of resistors in series with the diode, the case with two emitters for planar field emission, and cylindrical diodes. Ágúst Valfells and Kristinn Torfason worked on appropriate modelling of thermoelectric emission with Abhijit Jassem, who was visiting from the University of Michigan to learn about the MD code. The BS student Hákon Valur Haraldsson carried on with calculations of charge bunching in cylindrical vacuum diodes as well as working on his final project concerning space-charge shielding between neighboring field emitters. This work will continue in early 2018 in preparation for a journal publication. Hákon Örn Árnason has begun work on preparation of photoemitters for an experiment to see if THz radiation can be generated using the space-charge bunching mechanism as suggested in our previous theoretical work. Hákon Örn constructed GaAs cathodes with patterned Au masking that are likely to be an improvement on the Au cathodes with Pt masking as envisioned in the original experimental concept. Hákon Örn will begin his PhD studies with the group in 2018. Ágúst Valfells has worked on identifying applications and extensions to the MD code. A white paper has been submitted to the US Air Force Office of Scientific Research to propose funding for work on the aforementioned extensions and applications.

Comparison of different numerical methods for self-energy calculations.
Gunnar Þorgilsson and Sigurður I. Erlingsson are working on a project where different methods for calculating self-energies are compared. The self-energy is central quantity that is required to calculate transport in the scattering formalism. There is no clear consensus in the literature about which method is the fastest numerically. The goal of this project is to compare the different methods and the standard physics based methods to the more mathematical problem of solving quadratic matrix equations. A manuscript is in preparation.

Grants and other financial resources

Perovskites for photovoltaic efficient conversion technology, The Romanian/EEA Research Programme, Project EEA-JRP-RO-NO-2013-1-0116, PI Ioana Pintilie (National Institute of Materials Science, Romania), RU team leader Andrei Manolescu, total funds 1.25 mil. EUR, RU budget 82589 Euro, 2014-2017, funded by EEA. Ended in April 2017.

High photoconductive oxide films functionalized with GeSi nanoparticles for environmental applications (PhotoNanoP) M-ERA.NET project 2016-2019, in collaboration collaboration with National Institute of Materials Physics from Romania. RU team leader Halldór Svavarsson, RU budget 108000 Euro.

Core-shell nanoantennas, The Icelandic Research Fund, PI Andrei Manolescu, 41.3 mil. ISK (2016-2019).

DC vacuum-microdiode arrays as tunable THz sources, PI Ágúst Valfells, 44.9 mil. ISK (2017-2020)

Vacuum electronics, postdoctoral fellowship Kristinn Torfason, 24.5 mil ISK (2017-2020)

Use of silicon nanowires for electricity production from solar light, Landvirkjun project grant. PI Halldór Svavarsson, 3 mil ISK (2016-2017)

Solar simulator for characterization of solar cells, equipment funded by Infrastructure Fund of Rannis. Grant amount 2.2 mil ISK.

Funds from individual research accounts provided by the School of Science and Engineering were used for travel to conferences, for guest scientists, for new computers, and for software license.

Events related to the activity of the center (short visits, presentations, theses, etc.)

10-25 February, visit of Prof. Llorenc Serra from University of Balearic Islands, Mallorca, Spain, within the collaboration on Majorana physics in prismatic nanowires and spin-orbit interaction.

14 May, Ágúst Valfells gives the talk *"*Molecular Dynamics for Simulation of Vacuum Nanoelectronics.*"*, at DINAMO cnference, Siglufjörður, Iceland, 14-19 May 2017.

18 May, Andrei Manolescu gives the talk "Electron localization and optical absorption in prismatic shell structures", at DINAMO conference, Siglufjörður, Iceland, 14-19 May 2017.

20 May, Anna Sitek gives a talk entitled "Majorana states in prismatic core-shell nanowires" at the conference "Majorana states in condensed matter: towards topological quantum computation", Mallorca, Spain, 14-20 May 2017.

28 June, invited talk by Andrei Manolescu, "Localization of electrons in core-shell nanowires", at National Technical University, Taipei, Taiwan.

6 July, Anna Sitek, gives an invited talk entitled "Controlled Coulomb effects in core-shell quantum rings" at the conference ICTON 2017, Girona, Spain, 2-6 July 2017.

13 July, Andrei Manolescu, invited talk "Localization of electrons in core-shell nanowires", the 9-th International Conference on Advanced Materials ROCAM, Bucharest, 10-14 July.

14 August, Prof. Tom Antonsen from University of Maryland, visits the Nanophysics Center and gives the talk entitled Reciprocity and Adjoint Methods in Charged Particle Dynamics.

25 August – 4 September, Visit of Abhijit Jassem, PhD student at University of Michigan, Department of Nuclear Engineering, for training in using the vacuum electronics computer code written by Kristinn Torfason.

31 August – 20 September, visit of Cahit Kargi, Master student from Koc University, Istanbul, Turkey.

6-7 September, meeting at RU with the Romanian collaborators on the M-ERA.NET project "High photoconductive oxide films functionalized with GeSi nanoparticles for environmental applications".

5-12 November, visit of Prof. Carlos Egues, to work on the magnetoresistance project.

14 September, Taha Sultan has a presentation of his recent results on SiGe nanoparticles for the Romanian collaborators at the IEEE International Semiconductor Conference - CAS 2017, Sinaia, Romania.

18 October, Sigurður Erlingsson has his inaugural talk as a full Professor at RU.

20 November, Andrei Manolescu, invited talk "Localization of electrons and Majorana states in tubular nanowires", Institute of Theoretical Physics, Saclay, France.

Journal papers (e-prints, accepted, or published)

M. Nita, M. Tolea, D. C. Marinescu, A. Manolescu, Hund and anti-Hund rules in circular molecules, to appear in Phys. Rev. B **96**, 235101 (2017), arXiv:1711.06001.

V. Gudmundsson, N. R. Abdullah, A. Sitek, H.-S. Goan, C.-S. Tang, A. Manolescu, Electroluminescence caused by the transport of interacting electrons through parallel quantum dots in a photon cavity, Annalen der Physik, DOI: 10.1002/andp.201700334, arXiv:1706.03483, (2017).

A. Slav, C. Palade, I. Stavarache, V. S. Teodorescu, M. L. Ciurea, R. Müller, A. Dinescu, M. T. Sultan, A. Manolescu, J. T. Gudmundsson, H. G. Svavarsson, Influence of preparation conditions on structure and photosensing properties of GeSi/TiO2 multilayers, CAS 2017 Sinaia (Romania), IEEE Xplore Digital Library http://ieeexplore.ieee.org/document/8101154/ pp. 63-66 (2017).

G. Thorgilsson, S. I. Erlingsson, A. Manolescu, Thermoelectric current in tubular nanowires in transverse electric and magnetic fields, EDISON 20 Conference 2017, Journal of Physics: Conf. Series **906**, 012021 (2017).

V. Gudmundsson, N. R. Abdullah, A. Sitek, H. S. Goan, C. S. Tang, A. Manolescu, Current correlations for the transport of interacting electrons through parallel quantum dots in a photon cavity, submitted for publication, arXiv:1707.08295 (2017).

A. Manolescu, A. Sitek, J. Osca, L. Serra, V. Gudmundsson, T. D. Stanescu, Majorana states in prismatic core-shell nanowires, Phys. Rev. B **96**, 125435 (2017) arXiv:1705.04950.

S. I. Erlingsson, A. Manolescu, G. A. Nemnes, J. H. Bardarson, D. Sanchez, Reversal of thermoelectric current in tubular nanowires, Phys. Rev. Lett. **119**, 036804 (2017) arXiv:1705.01569.

A. Sitek, M. Urbaneja Torres, K. Torfason, V. Gudmundsson, A. Manolescu, Controlled Coulomb effects in core-shell quantum rings, ICTON 2017 Girona, IEEE Xplore Digital Library http://ieeexplore.ieee.org/document/8025179/ pp. 1-4, arXiv:1704.06136 (2017).

P. Zhang, A. Valfells, L.K. Ang, J.W. Luginsland, and Y.Y. Lau, 100 Years of the Physics of Diodes, Applied Physics Reviews, **4**, 011304 (2017).

N. Plugaru, G. A. Nemnes, L. Filip, I. Pintilie, L. Pintilie, K. T. Butler, A. Manolescu, Atomistic Simulations of methylammonium lead halide layers on PbTiO3 (001) surfaces, J. Phys. Chem. C **121**, 9096 (2017).

G. A. Nemnes, C. Besleaga, V. Stancu, D. E. Dogaru, L. N. Leonat, L. Pintilie, K. Torfason, M. Ilkov, A. Manolescu, I. Pintilie, Normal and inverted hysteresis in perovskite solar cells, J. Phys. Chem. C 121, 11207 (2017), arXiv:1704.03300**.**

G. A. Nemnes, C. Besleaga, A. G. Tomulescu, I. Pintilie, L. Pintilie, K. Torfason, A. Manolescu, Dynamic electrical behavior of halide perovskite based solar cells, Solar Energy Materials & Solar Cells 159, 197 (2017), arXiv:1606.00335.

A. Sitek, M. Tolea, M. Nita, L. Serra, V. Gudmundsson, A. Manolescu, In-gap corner states in core-shell polygonal quantum rings, Scientific Reports **7**, 40197 (2017).

V. Gudmundsson, T. H. Jonsson, A. L. Bernodusson, N. R. Abdullah, A. Sitek, H.-S. Goan, C.-S. Tang, A. Manolescu, Regimes of radiative and nonradiative transitions in transport through an electronic system in a photon cavity reaching a steady state, Annalen der Pysik, **529**, 1600177 (2017), arXiv:1605.08248.

V. Gudmundsson, N. R. Abdullah, A. Sitek, H.-S. Goan, C.–S. Tang, A. Manolescu, Time-dependent current into and through multilevel parallel quantum dots in a photon cavity, Phys. Rev. B **95**, 195307 (2017), arXiv:1611.09453.

G. A. Nemnes, C. Visan, A. Manolescu, Electronic and thermal conduction properties of halogenated porous graphene nanoribbons, Journal of Materials Chemistry C **5**, 4435 (2017), arXiv:1612.07949.

T. H. Jonsson, A. Manolescu, H.-S. Goan, N. R. Abdullah, A. Sitek, C.-S. Tang, V. Gudmundsson, Efficient determination of the Markovian time-evolution towards a steady-state of a complex open quantum system, submitted to publication, Computer Physics Communications **220**, 81–90 (2017), arXiv:1610.03223.

See also http://nano.ru.is/publications

Contributions to conferences

K. Torfason, A. Manolescu, A. Valfells, A. Jassem, Molecular Dynamics Based Investigation of Contribution of Discrete Particle Effects Near Cathode to Beam Emittance, ICOPS 2015, Atlantic City, New Jersey, USA, May 21-25 2017.

I. Pintilie, C. Besleaga, L.E. Abramiuc, V. Stancu, A.G. Tomulescu, M. Sima, L. Leonat, L. Trinca, D.A. Dogaru, N. Plugaru, L. Pintilie, G.A. Nemnes, A. Manolescu, Hysteresis effects and stability issues in perovskite solar cells, The 9th International Conference on Advanced Materials ROCAM, Bucharest, 10-14 July 2017, http://rocam.unibuc.ro/rocam2017/

S. I. Erlingsson, A. Manolescu, G. A. Nemnes, J. H. Bardarsson, D. Sanchez, Reversal of thermoelectric current in tubular nanowires, Nanowire Week, Lund, 29 May - 2 June 2017
http://www.nanowireweek.lu.se/home/

A. Manolescu, A. Sitek, L. Serra, T. D. Stanescu, Majorana states in core-shell nanowires with polygonal cross section, Nanowire Week, Lund, 29 May - 2 June 2017,
http://www.nanowireweek.lu.se/home/

M. Urbaneja Torres, A. Sitek, V. Gudmundsson, A. Manolescu, Coulomb interaction effects on polygonal core-shell nanowires, Nanowire Week, Lund, 29 May - 2 June, 2017,
http://www.nanowireweek.lu.se/home/

A. Sitek, K. Torfason, M. Urbaneja Torres, V. Gudmundsson, A. Manolescu, Excitons in core-shell quantum rings, Nanowire Week, Lund, 29 May - 2 June, 2017, http://www.nanowireweek.lu.se/home/

G. A. Nemnes, T. L. Mitran, A. Manolescu, D. Dragoman, Electric control of the effective doping in boron/nitrogen substituted bilayer graphene, The 2017 E-MRS Fall Meeting, Warsaw, 18-20 September http://www.european-mrs.com/meetings/2017-fall-meeting

G. A. Nemnes, C. Besleaga, V. Stancu, D. E. Dogaru, L. N. Leonat, L. Pintilie, K. Torfason, M. Ilkov, A. Manolescu, I. Pintilie, Normal and inverted hysteresis in perovskite solar cells, ICSS San Sebastian 9-13 May 2017, http://emnmeeting.org/Europe/wp-content/uploads/2017/04/ICSSEMN-Nanoparticles-Final-Program.pdf

G. A. Nemnes, C. Besleaga, V. Stancu, A. Palici, D. E. Dogaru, L. N. Leonat, L. Pintilie, K. Torfason, M. Ilkov, D. V. Anghel, I. Pintilie, A. Manolescu, Modeling hysteretic effects in perovskite solar cells, MMCP Dubna 3-7 July, https://indico.jinr.ru/contributionDisplay.py?contribId=79&sessionId=11&confId=137

R. Chirla, C.D. Horea, T.O. Costea, R. Dragomir, A. Manolescu, C.P. Moca, AIP Conference Proceedings 1796, 030002 (2017) (TIM15-16 Timisoara), http://aip.scitation.org/doi/pdf/10.1063/1.4972367

Research plans for 2018

TiO_2 thin films with embedded GeSi particles: fabrication, optical, and electrical characterization.

Polarization of Majorana states in core-shell nanowires.

Thermoelectric transport in core-shell nanowires.

Core-shell nanoantennas: electromagnetic absorption and plasmons

Vacuum electronics: Experiment on THz generation. Discrete particle effects and the role of surface inhomogeneity in microgap breakdown. Origins of emittance. Optimize the code to run on a GPU. Have Abhijit use the code to study thermionic emission and surface inhomogeneity's. Circuit elements will be added to the code.

Mechanical properties of Silicon nanowires (SiNWs): bending and vibrations, theoretical simulations and experimental investigations.

It is planned to make experimental tests with core-shell SiNWs in cooperation with National Institute for Research and Development in Microtechnologies – IMT, in Romania with the aim of improving broadband optical absorption and reduce radial carrier collection distances in solar cell devices. The core-shell SiNWs will be obtained by covering SiNWs with transparent and conductive oxide.

Topological insulators: Transport in topological insulator and superconductor heterostructures. Magnetic impurities in topological insulators, transport and optical properties.