Computational Methods for Nanosystems

Course description sheet

Basic information

Field of study AGH UST International Courses **Major** All **Organisational unit** Generic subjects **Study level** any level **Form of study** Full-time studies **Profile** General academic	**Didactic cycle** 2021/2022 **Course code** POGJOS.A200000O.60766ec4329b9.21 **Lecture languages** english **Mandatoriness** Elective **Block** General Modules **Course related to scientific research** Yes **USOS code** 693-INTCOURSE-xS-210

Course coordinator	Michał Zegrodnik
Lecturer	Michał Zegrodnik, Andrzej Biborski

Period Summer semester	**Method of verification of the learning outcomes** Exam **Activities and hours** Workshop classes: 30	**Number of ECTS credits** 4

Goals

C1	The principal purpose of the module is to provide students with basic knowledge and skills in the modelling of nano-systems both from the perspective of theoretical description and numerical calculations carried out on a computer with the use of Kwant library (https://kwant-project.org/). Exemplary project realized within the classes is available under the following link: http://acmin.agh.edu.pl/didactics/CompNano/modelling_QPC.html

Course's learning outcomes

Code	Outcomes in terms of	Learning outcomes prescribed to a field of study	Methods of verification
Knowledge – Student knows and understands:			
W1	the quantum mechanical description of various nanosystems and how they are realized using semiconducting materials.		Examination
W2	the description of electron transport through nanodevices (also in the presence of magnetic field) and related effects such as conductance quantization, negative differential resistance, Hall effect, and Aharonov-Bohm effect.		Examination
Skills – Student can:			
U1	model various nano-systems and predict their features within the framework of non-commercial calculation package(s) such as KWANT.		Activity during classes, Project
U2	apply numerical methods to quantum mechanical problems: discretization, diagonalization, integration etc.		Activity during classes, Project

Program content ensuring the achievement of the learning outcomes prescribed to the module

The classes will cover necessary theoretical formalism and computer laboratory exercises. The emphasis will be placed on discussing the principal experimental effects in the field of physics of nanostructures and then carrying out numerical calculations on a computer which reproduce the given physical effect. Selected problems are to be solved by the students as calculation projects with the use of the Kwant package (https://kwant-project.org/). Exemplary project realized within the classes is available under the following link: http://acmin.agh.edu.pl/didactics/CompNano/modelling_QPC.html

Student workload

Activity form	Average amount of hours* needed to complete each activity form
Workshop classes	30
Preparation for classes	15
Examination or final test/colloquium	2
Contact hours	15
Preparation of project, presentation, essay, report	20
Realization of independently performed tasks	20
Student workload	**Hours** 102

Workload involving teacher	**Hours** 30

* hour means 45 minutes

Program content

No.	Program content	Course's learning outcomes	Activities
1.	Schrodinger equation, quantum size effect (quantum wells, quantum dots and quantum wires, two-dimensional electron gas), elements of band theory, effective mass approximation, semiconductor heterostructures.	W1, U1, U2	Workshop classes
2.	Description of electron transport through nanostructures (ballistic transport and diffusive transport, transmission coefficient, Landauer Formula, Tsu-Esaki model, quantum point contact and resonant tunneling diode); Electron transport in the presence of magnetic field (Landau levels, quantum Hall effect, quantum rings and Aharonov-Bohm effect);	W2, U1, U2	Workshop classes
3.	Basics of python programming language and KWANT simulation package.	U1, U2	Workshop classes

Extended information/Additional elements

Teaching methods and techniques:

Discussion, Case study, Project based learning

Activities	Methods of verification	Credit conditions
Workshop	Activity during classes, Project, Examination	

Method of determining the final grade

workshop classes (active participation in classes and project realization) - 60% of the final grade , exam - 40% of the final grade.

Prerequisites and additional requirements

Basic knowledge in quantum mechanics:
- Schroedinger equation, wave function
- quantization of physical quantities (energy, angular momentum etc.)

Literature

Obligatory

1. Yuli V. Nazarov, Yaroslav M. Blenter, "Quantum transport Introduction to Nanoscience", Cambridge University Press 2009
2. Supriyo Datta, "Quantum Transport: Atom to Transistor", Cambridge University Press, 2005
3. C.W.J.Beenakker, H.van Houten, "Quantum Transport in Semiconductor Nanostructures", Solid State Physics, Volume 44, 1991, Pages 1-228
4. C. Kittel, "Wstęp do fizyki ciała stałego", Warszawa : Państwowe Wydawnictwo Naukowe, 1976.
5. Neil W. Ashcroft, N. David Mermin , "Fizyka ciała stałego", Warszawa : Państwowe Wydawnictwo Naukowe, 1986
6. J. Spalek, "Wstęp do fizyki materii skondensowanej", Warszawa: Państwowe Wydawnictwo Naukowe 2015

Scientific research and publications

Publications

1. Dot-ring nanostructure: Rigorous analysis of many-electron effects, A. Biborski, A. P. Kądzielawa, A. Gorczyca-Goraj, E. Zipper, M. M. Maśka and J. Spałek, Scientific Reports 6, 29887 (2016), http://dx.doi.org/10.1038/srep29887
2. Tunneling conductance through the half-metal/conical magnet/superconductor junctions in the adiabatic and non-adiabatic regimes: Self-consistent calculations, P.Wójcik, M.Zegrodnik, B.Rzeszotarski, J.Adamowski, Physica E: Low-dimensional Systems and Nanostructures 83, 466 (2016), https://doi.org/10.1016/j.physe.2015.12.021
3. Interplay between quantum confinement and Fulde–Ferrell–Larkin–Ovchinnikov phase in superconducting nanofilms, P. Wójcik, M. Zegrodnik, Physica E 83, 442-449 (2016), http://dx.doi.org/10.1016/j.physe.2016.01.020
4. Fulde-Ferrell state induced by the orbital effect in a superconducting nanowire, P. Wójcik, M. Zegrodnik, J. Spałek, PHYSICAL REVIEW B 91, 224511 (2015), http://dx.doi.org/10.1103/PhysRevB.91.224511
5. Orbital effect on the in-plane critical field in free-standing superconducting nanofilms, P. Wójcik, M. Zegrodnik, Physica Status Solidi B 252, 2096-2103 (2015), http://dx.doi.org/10.1002/pssb.201552067