SYLLABUS

1. Information regarding the program

1.1 Higher education institution	Babeş-Bolyai University
1.2 Faculty	Faculty of Physics
1.3 Department	Doctoral School of Physics
1.4 Field of study	Physics
1.5 Study cycle	Doctorate
1.6 Study program / Qualification	Doctoral training/PhD in Physics

2. Course data

2.1 Name of discipline			Theoretical and computational methods in solid state physics				
2.2 Teacher responsible for lectures			CS II dr. Diana Benea, Prof. dr. Ioan Grosu, Prof. dr. Coriolan Tiușan				
2.3 Teacher responsible for seminars			CS II dr. Diana Benea, Prof. dr. Ioan Grosu, Prof. dr. Coriolan Tiușan				
2.4 Year of study	I	**2.5 Semester**	I	**2.6 Type of evaluation**	E	**2.7 Course framework**	DS

3. Estimated total time of teaching activities (hours per semester)

3.1 Hours per week	3	Out of which: 3.2 Lectures	2	3.3 Seminars / Laboratory classes	1
3.4 Total hours in the curriculum	36	Out of which: 3.5 Lectures	24	3.6 Seminars / Laboratory classes	12
Allocation of study time:					**89**
Study supported by textbooks, other course materials, recommended bibliography and personal student notes					34
Additional learning activities in the library, on specialized online platforms and in the field					24
Preparation of seminars/laboratory classes, topics, papers, portfolios and essays					15
Tutoring					12
Examinations					4
Other activities					–

3.9 Total individual study hours	89
3.10 Total hours per semester	125
3.11 Number of ECTS credits	10

4. Prerequisites (if necessary)

4.1 Curriculum	Quantum mechanics, Statistical physics, Physics of atoms and molecules, Numerical methods, Calculus, Algebra
4.2 Competences	- computational skills, - introductory methods of theoretical physics

5. Conditions (where applicable)

5.1 Conducting lectures	Course hall, appropriate board, projector, dedicated software, computer
5.2 Conducting seminars/laboratory classes	Course hall, appropriate board, projector, dedicated software, computer network

6. Specific competences acquired

Professional competences	C1. Use of advanced knowledge of physics, mathematics and chemistry of solids for studies in condensed state physics and materials science. The ability to analyze and synthesize physical data, the ability to model complex phenomena. C2. Capitalizing on the physical fundamentals, methods and tools of solid state physics and materials science for specific production, expertise and monitoring activities. Acquiring a multi- and interdisciplinary way of thinking. C3. Planning and conducting experiments to assess uncertainty and interpret results. Use of laboratory equipment for basic research, equipment and industrial laboratories for conducting research experiments. Planning and implementing independent experiments or experimental investigations and evaluating the results C4. Communicating complex scientific ideas, conclusions or results of a scientific experiment. The ability to obtain and argue scientific results, the ability to produce scientific papers and to liaise with the editorial board of scientific journals in the field. Identification and appropriate use of the main physical laws and principles in a given context.

Transversal competencies	CT1. Carrying out professional tasks efficiently and responsibly in compliance with the legislation and deontology specific to the field under qualified assistance. Responsible performance of professional duties in terms of self-assessment decision-making. CT2. Effective work in multidisciplinary teams on various hierarchical levels. Identification of roles and responsibilities in a team and the application of communication techniques and effective work within the team, based on dialogue, positive attitude, mutual respect, diversity and multiculturalism as well as a continuous improvement of the activity. CT3. Effective use of information sources and communication resources and assisted professional training, both in Romanian and in an international language. Identification of opportunities for continuous training and effective utilization of learning resources and techniques for personal development and adaptation to the requirements of the labor market.

7. Course objectives (based on the acquired competencies grid)

7.1 The general objective of the discipline	- Acquisition of theoretical and computatonal notions regarding the use of advanced methods in the study of the condensed state
7.2 Specific objectives	- Acquisition of notions related to: - Writing in the second quantification of a series of operators and groups of operators. - Using the method of the equation of motion to determine the energy spectrum, in the case of systems of many particles with interactions. - Determination of some properties of many-particle systems, in the Hartree and Hartree-Fock approximations. - Determination of electrical/magnetic properties of solids based on their crystalline structure - Determination of some spectroscopic properties of solids based on their crystalline structure - Establishing correlations between theoretical calculations and experimental data.

8. Content

8.1 Lectures	**Teaching methods**	**Comments**
1. Introduction to Density Functional Theory. Principles. The Kohn-Sham equation. Local density approximation. Electronic structure of solids. Multiple	Interactive lecture, Directed discussion, debate, Case-based	4 hours

scattering theory (Korringa-Kohn-Rostocker). Green functions. Calculating observables.	learning, Just-in-time teaching	
2. Ab-inito methods for describing the magnetic/spectroscopic properties of solids: Compton scattering, positron annihilation, magnetic dichroism in X-ray absorption, XPS spectroscopy, the Heisenberg model for exchange coupling.		4 hours
3. The second quantization, fermions and bosons. Operators in the second quantization, the two-particle interaction.		3 hours
4. Representations. The method of the equation of motion. Hartree and Hartree-Fock approximations		5 hours
5. Simple quantum models applied in surface science, nano-magnetism and spintronics: the Stoner Hamiltonian, the Rahba Hamiltonian and spin manipulation in electric fields, the Rashba-Stoner Hamiltonian spin precession in electric field and voltage controlled magnetic anisotropy.		4 hours
6. Micromagnetic and atomistic modeling of magnetic systems, nano and heterostructures.		2 hours
7. Exact diaginalization of 1D and 2D quantum systems: single spin NMR manipulation, Ising chains, 2D lattices, quantum skyrmions and quantum gates with skyrmionic qubits.		2 hours
8.2 Seminars / laboratory classes	**Teaching methods**	**Comments**
1. Self-consistent calculations of the electronic band structure for selected systems. Calculation of the density of states. Dispersion relation and Bloch spectral functions. Calculation of the photoemission spectrum in the valence band. Calculation of exchange coupling parameters for different magnetic systems. Stability of spine structures.	Problem based learning, Project based learning, Inquiry guided learning, Experiential learning	4 hours
2. Operators in the second quantization, the two-particle interaction.		4 hours
3. Photoemission/angle resolved photoemission spectoscopy and Datta and Dass spin transistor		1 hour

4. Macrospin LLG for magnetization dynamics: electric field magnetization manipulation in magnetic tunnel junctions		1 hour
5. VAMPIRE (atomistic) and Mumax3 (micromagnetic) modelling of chiral magnetic structures, skyrmions		1 hour
6. ED examples using Quspin package for NMR precession of single spin and Ising chains		1 hour

Bibliography

1. SPRKKR manual – H. Ebert , LMU Munich 2017 (http://ebert.cup.uni-muenchen.de)
2. Structura electronica de benzi cu aplicatii in solide, D. Benea 2014 (lucrari de laborator).
3. P. Strange, Relativistic Quantum Mechanics (Cambridge University Press, 1998).
4. H. Ebert, J. Minar, and D. Kodderitzsch, Rep. Prog. Phys. 74, 096501 (2011).
5. A. I. Liechtenstein,M. I. Katsnelson, V. P. Antropov, and V. A. Gubanov, J.Magn.Magn. Materials 67, 65 (1987).
6. U. Mizutani, Introduction to the Electron Theory of Metals,Cambridge University Press 2001.
7. D. Pines, P. Nozieres, "The Theory of Quantum Liquids", vol.I, Benjamin, New York, (1966)
8. I.Tifrea, I.Grosu, M.Crisan, "Metode cuantice pentru studiul sistemelor cu multe particule. Aplicatii la sisteme fermionice si bosonice", Presa Universitara Clujeana, (2005)
9. I.Grosu, I.Tifrea, "Teoria materiei condensate. Probleme", Casa Cartii de Stiinta, Cluj, (2006)
10. Barnes, S., Ieda, J. & Maekawa, S. Rashba Spin-Orbit Anisotropy and the Electric Field Control of Magnetism. *Sci Rep* **4**, 4105 (2014). https://doi.org/10.1038/srep04105.
11. J. M. D. Coey, Magnetism and Magnetic Materials, Cambridge University Press (2010), ISBN: 9780511845000.
12. R. Feynman, The Feynman Lectures on Physics, Vol. III: The New Millennium Edition: Quantum Mechanics, ISBN 0465023827, 9780465023820.
13. E.I. Rashba, Fiz. Tverd. Tela S.-Peterburg 2, 1224 (1960) Sov. Phys. Solid State 2, 1109 1960; Yu. A. Bychkov and E.I. Rashba, Pis'ma Zh. Eksp. Teor. Fiz. 39, 66 1984 JETP Lett. 39, 78 (1984).

9. Aligning the contents of the discipline with the expectations of the epistemic community, representatives, professional associations and standard employers operating in the program field

The content of the discipline is in line with what is studied in other university centers in the country and abroad. In order to adapt to the requirements imposed by the labor market, the content of the discipline was harmonized with the requirements imposed by the specifics of postgraduate education, research institutes and the business environment.

10. Examination

Activity type	10.1 Evaluation criteria	10.2 Evaluation methods	10.3 Weight in the final grade
10.4 Lectures	Assessment of knowledge	Written exam	75%
10.5 Seminars / laboratory classes	Activity during seminars	Discussions, answers to questions	25%
10.6 Minimum performance standard			
Choosing a computational and a theoretical method for a certain kind of characterization.			

Signature of course n	Signature of seminar coordinator
CS II. dr. Diana Benea	CS II dr. Diana Benea
Prof. dr. Ioan Grosu	Prof. dr. Ioan Grosu
Prof. dr. Coriolan Tiușan	Prof. dr. Coriolan Tiușan

Date	Signature Head of department
21.09.2024	Prof. dr. Vasile Chiș