Federal State Autonomous Educational Institution of Higher Education "Moscow Institute of Physics and Technology (National Research University)"

APPROVED
Head of Landau Phystech-School of Physics & Research
A.V. Rogachev

Work program of the course (training module)

course:	First Principles Simulations and Modeling/Первопринципные методы расчета свойств материалов
major:	Photonics and Optical Informatics
specialization:	Photonics, Quantum Technologies & 2D Materials/Фотоника, квантовые технологии и двумерные материалы
	Landau Phystech-School of Physics & Research
	Chair of Physics and Technology of nanostructures
term:	2
qualification:	Master

Semester, form of interim assessment: 3 (fall) - Exam

Academic hours: 30 AH in total, including:
- lectures: 30 AH.
- seminars: 0 AH.
- laboratory practical: 0 AH.

Independent work: 30 AH.

Exam preparation: 30 AH.

In total: 90 AH, credits in total: 2

Author of the program: N.L. Matsko, candidate of physics and mathematical sciences

The program was discussed at the Chair of Physics and Technology of nanostructures 20.05.2021

Annotation

The course will present methods for predicting the crystal structure of materials and calculating their properties. Also will be solved model problems to calculate the electronic band structure and density of states, phonon properties, superconducting properties, etc. for some materials. To model large systems, molecular dynamics methods will be described and interatomic potentials based on machine learning will be presented. The course aims to familiarize students with the peculiarities of calculations in multielectronic systems. The methodology of calculations, the limitations of various approaches are reviewed, and the concept of elementary excitations in the system and correlation energy is introduced. The question of optical excitations in a system of many electrons is studied. The following topics will be studied: Mean Field Theory. The Hartree-Fock method and first corrections to it. Electron density functional theory, exchange-correlation potential. Limitations of mean field theories. Optical absorption spectra, plasmons, excitons, features of electronic spectra. Correlation energy. Properties of electron gas. RPA model. Green's function. Diagramming technique as applied to solids. Response function of the system. Frequency dependent polarizability and dielectric function. GW, DFT+U, Configurational Interaction, TDDFT approximations.

1. Study objective

Purpose of the course

To form an idea of the features of calculations in multielectronic systems.

Tasks of the course

Familiarity with the methodology of calculations, understanding the limitations and limits of the applicability of different approaches. Acquaintance with the concept of elementary excitations in the system, correlation energy. Introduction to optical excitations in a system of many electrons.

2. List of the planned results of the course (training module), correlated with the planned results of the mastering the educational program

Mastering the discipline is aimed at the formation of the following competencies:

Code and the name of the competence	Competency indicators
Gen.Pro.C-1 Gain fundamental scientific knowledge in the field of physical and mathematical sciences	Gen.Pro.C-1.1 Apply fundamental scientific knowledge in the field of physical and mathematical sciences
	Gen.Pro.C-1.2 Able to summarise and critically evaluate experiences and research results in the field of photonics and opto-informatics
	Gen.Pro.C-1.3 Understands the interdisciplinary links in mathematics and physics and is able to apply them to problems in photonics and opto-informatics
Gen.Pro.C-2 Acquire an understanding of current scientific and technological challenges in professional settings, and scientifically formulate professional objectives	Gen.Pro.C-2.3 Understand professional terminology used in modern scientific and technical literature and present scientific results in oral and written form within professional communication
Gen.Pro.C-3 Select and/or develop approaches to professional problem-solving with consideration to the limitations and specifics of different solution methods	Gen.Pro.C-3.1 Analyze problems, plan research strategy to achieve solution(s), propose, and combine solution approaches
	Gen.Pro.C-3.2 Employ research methods to solve new problems, and apply knowledge from various fields of science (technology)
	Gen.Pro.C-3.3 Gain knowledge of analytical and computational methods of problem-solving, understand the limitations for applying the obtained solutions in practice
Gen.Pro.C-4 Successfully perform a task, analyze the results and present conclusions, apply knowledge and skills in the field of physical and mathematical sciences and ICTs	Gen.Pro.C-4.2 Apply knowledge in the field of physical and mathematical sciences to solve problems, make conclusions, and evaluate the obtained results
	Gen.Pro.C-4.3 Justify the chosen method of scientific research
Pro.C-1 Assign, formalize, and solve tasks	Pro.C-1.1 Locate, analyze, and summarize information on current research findings within a selected subject field

Pro.C-1 Assign, formalize, and solve tasks, develop and research mathematical models of the studied phenomena and processes, systematically analyze scientific problems and obtain new scientific results	Pro.C-1.2 Make hypotheses, build mathematical models of the studied phenomena and processes, evaluate the quality of the developed model
	Pro.C-1.3 Able to apply theoretical and/or experimental research methods in photonics and opto-informatics to a specific scientific problem and interpret the results obtained
Pro.C-2 Organize and conduct scientific research and testing independently or as a member (leader) of a small research team	Pro.C-2.1 Able to plan and carry out research in photonics and opto-informatics independently or as part of a research team
	Pro.C-2.2 Conduct tests of research results through scientific publications and participation in conferences

3. List of the planned results of the course (training module)

As a result of studying the course the student should:

know:

The concept of correlation energy, the concepts of elementary excitations in a system of many electrons.

be able to:

Evaluate electron-electron interaction effects; evaluate the effect of many-electron effects on the optical properties of a system.

master:

Fundamentals of numerical methodology in many-electron systems.

4. Content of the course (training module), structured by topics (sections), indicating the number of allocated academic hours and types of training sessions

4.1. The sections of the course (training module) and the complexity of the types of training sessions

№	Topic (section) of the course	Types of training sessions, including independent work			
		Lectures	Seminars	Laboratory practical	Independent work
1	The theory of the mean self-consistent field	2			2
2	Coulomb interaction shielding and plasmons in metals	2			2
3	Electron-optical excitations	2			2
4	Many-Body Perturbation Theory	4			4
5	Numerical packages for calculations within the mean self-consistent field method and beyond	8			8
6	The Green's function	2			2
7	Typical diagrams in solids. The GW method	2			2
8	System response	2			2
9	The DFT+U method	6			6
AH in total		30			30
Exam preparation		30 AH.			
Total complexity		90 AH., credits in total 2			

4.2. Content of the course (training module), structured by topics (sections)

Semester: 3 (Fall)

1. The theory of the mean self-consistent field

Introduction. Problem statement. The theory of the average self-consistent field. The Hartree and Hartree-Fock equations. The theory of the electron density functional. The main limitations of these approaches.

2. Coulomb interaction shielding and plasmons in metals

The Hartree-Fock approximation as the first order of perturbation theory. Screening of the Coulomb interaction in an electron gas. The long-range effect of the Coulomb interaction. Long-wave density perturbations, plasmons, and the RPA approximation.

3. Electron-optical excitations

Pairing of the electromagnetic wave with surface plasmons. Surface Plasmon Polariton. Surface plasmons on a structured surface.

4. Many-Body Perturbation Theory

The Green function and the basics of diagram technique. Diagram decomposition of the Green's function.

5. Numerical packages for calculations within the mean self-consistent field method and beyond

Quanyum Espresso, VASP, BerkeleyGW, Octopus.

6. The Green's function

Free Green's function. The total Green function. Dyson's equation. Actually energy part. The vertex part. Spectral representation of the Green's function. A quasi-partical description of an electronic system.

7. Typical diagrams in solids. The GW method

The Hedin equations. The GW method. Plasma pole approximation.

8. System response

Definition. Causality. Kramers-Kronig relations. The system response function.

9. The DFT+U method

"Re-localization" of electrons in DFT. Mottov insulators. The Hubbard model. DFT+U (LDA+U).

5. Description of the material and technical facilities that are necessary for the implementation of the educational process of the course (training module)

A set of electronic presentations/slides; an audience equipped with presentation equipment (projector, screen, computer / laptop); if necessary, special technical means for students with disabilities and persons with disabilities.

6. List of the main and additional literature, that is necessary for the course (training module) mastering

Main literature

1. Фейнмановские диаграммы в проблеме многих тел [Текст]/Р. Д. Маттук, -М., Мир, 1969
2. Физика твердого тела [Текст] : в 2 т. Т. 1 / Н. Ашкрофт, Н. Мермин ; пер. с англ. А. С. Михайлова ; под ред. М. И. Каганова .— М. : Мир, 1979 .— 399 с.
3. Физика твердого тела [Текст] : в 2 т. Т. 2 : [учеб. пособие для вузов] / Н. Ашкрофт, Н. Мермин ; пер. с англ. К. И. Кугеля, А. С. Михайлова ; под ред. М. И. Каганова .— М. : Мир, 1979 .— 424 с.

Additional literature

1. Элементарные возбуждения в твердых телах [Текст]/Д. Пайнс , пер. с англ. Ю. В. Гуляева , -М., Мир, 1965

7. List of web resources that are necessary for the course (training module) mastering

Not used

8. List of information technologies used for implementation of the educational process, including a list of software and information reference systems (if necessary)

Demonstration of presentations, video conferences.

9. Guidelines for students to master the course

A student studying the discipline must, on the one hand, master the general conceptual apparatus, and on the other hand, must learn to apply theoretical knowledge in practice.
As a result of studying the discipline, the student must know the basic definitions and concepts, be able to apply the knowledge gained to solve various problems.
Successful completion of the course requires:
- attendance of all classes provided for by the curriculum for the discipline;
- keeping a synopsis of classes;
- student's intense independent work.

Independent work includes:
- reading recommended literature;
- study of educational material, preparation of answers to questions intended for independent study;
- solving problems offered to students in the classroom;
- preparation for the performance of tasks of the intermediate certification.

An indicator of mastery of the material is the ability to answer questions on the topics of the discipline without a synopsis.
It is important to achieve an understanding of the material being studied, not its mechanical memorization. If a student finds it difficult to study certain topics, questions, he/she should seek advice from a teacher.
Intermediate control of students' knowledge is possible in the form of solving problems in accordance with the topic of classes.

SUPPLEMENT

Assessment funds for course (training module)

major:	Photonics and Optical Informatics
specialization:	Photonics, Quantum Technologies & 2D Materials/Фотоника, квантовые технологии и двумерные материалы
	Landau Phystech-School of Physics & Research
	Chair of Physics and Technology of nanostructures
term:	2
qualification:	Master

Semester, form of interim assessment: 3 (fall) - Exam

Author: N.L. Matsko, candidate of physics and mathematical sciences

1. Competencies formed during the process of studying the course

Code and the name of the competence	Competency indicators
Gen.Pro.C-1 Gain fundamental scientific knowledge in the field of physical and mathematical sciences	Gen.Pro.C-1.1 Apply fundamental scientific knowledge in the field of physical and mathematical sciences
	Gen.Pro.C-1.2 Able to summarise and critically evaluate experiences and research results in the field of photonics and opto-informatics
	Gen.Pro.C-1.3 Understands the interdisciplinary links in mathematics and physics and is able to apply them to problems in photonics and opto-informatics
Gen.Pro.C-2 Acquire an understanding of current scientific and technological challenges in professional settings, and scientifically formulate professional objectives	Gen.Pro.C-2.3 Understand professional terminology used in modern scientific and technical literature and present scientific results in oral and written form within professional communication
Gen.Pro.C-3 Select and/or develop approaches to professional problem-solving with consideration to the limitations and specifics of different solution methods	Gen.Pro.C-3.1 Analyze problems, plan research strategy to achieve solution(s), propose, and combine solution approaches
	Gen.Pro.C-3.2 Employ research methods to solve new problems, and apply knowledge from various fields of science (technology)
	Gen.Pro.C-3.3 Gain knowledge of analytical and computational methods of problem-solving, understand the limitations for applying the obtained solutions in practice
Gen.Pro.C-4 Successfully perform a task, analyze the results and present conclusions, apply knowledge and skills in the field of physical and mathematical sciences and ICTs	Gen.Pro.C-4.2 Apply knowledge in the field of physical and mathematical sciences to solve problems, make conclusions, and evaluate the obtained results
	Gen.Pro.C-4.3 Justify the chosen method of scientific research
Pro.C-1 Assign, formalize, and solve tasks, develop and research mathematical models of the studied phenomena and processes, systematically analyze scientific problems and obtain new scientific results	Pro.C-1.1 Locate, analyze, and summarize information on current research findings within a selected subject field
	Pro.C-1.2 Make hypotheses, build mathematical models of the studied phenomena and processes, evaluate the quality of the developed model
	Pro.C-1.3 Able to apply theoretical and/or experimental research methods in photonics and opto-informatics to a specific scientific problem and interpret the results obtained
Pro.C-2 Organize and conduct scientific research and testing independently or as a member (leader) of a small research team	Pro.C-2.1 Able to plan and carry out research in photonics and opto-informatics independently or as part of a research team
	Pro.C-2.2 Conduct tests of research results through scientific publications and participation in conferences

2. Competency assessment indicators

As a result of studying the course the student should:

know:

The concept of correlation energy, the concepts of elementary excitations in a system of many electrons.

be able to:

Evaluate electron-electron interaction effects; evaluate the effect of many-electron effects on the optical properties of a system.

master:

Fundamentals of numerical methodology in many-electron systems.

3. List of typical control tasks used to evaluate knowledge and skills

Not provided.

4. Evaluation criteria

List of control questions:
1. Formulate the basic statements of the self-consistent field method
2. Elementary excitations in an electron gas. Plasmons and optical excitations.
3. Surface plasmons in metal and optical properties
4. Correlation energy.
5. Coulomb interaction shielding
6. Friedel oscillations

Examples of control assignments:
1. Write down Hartree-Fock equation and describe its main properties.
2. Formulate the general principles of the electron density functional theory
3. the basic properties of the dielectric response function in an electron gas
4. Find the plasma frequency in an electron gas
5. Write diagrams for Fock operators, exchange interaction, screening diagrams in chaotic phase model
6 Find optical spectra using the spectral representation of the Green's function

Examples of examination tickets:
Ticket 1.
1. Average self-consistent field theory.
2. The Hartree-Fock equation. The theory of the electron density functional.
Ticket 2.
1. Shielding and plasmons.
2. Electron-optical excitations.
Ticket 3.
1. Many-Body Perturbation Theory and the Green's Function.
2. Free Green's function. The total Green's function. Shielded Coulomb interaction.
Ticket 4.
1. The Green's function. Practical aspects. Typical diagram blocks. Diagrams of Hartree and Fock operators, RPA.
2. Optical spectra and spectral representation of the Green's function.
Ticket 5.
1. GW and DFT+U approximations.
2. Hartree-Fock equation. The theory of the electron density functional.
Ticket 6.
1. The concept of the system response function. Causality principle and Cramers-Kronig relations.
2. Dielectric function and inverse dielectric function.

Assessment “excellent (10)” is given to a student who has displayed comprehensive, systematic and deep knowledge of the educational program material, has independently performed all the tasks stipulated by the program, has deeply studied the basic and additional literature recommended by the program, has been actively working in the classroom, and understands the basic scientific concepts on studied discipline, who showed creativity and scientific approach in understanding and presenting educational program material, whose answer is characterized by using rich and adequate terms, and by the consistent and logical presentation of the material;

Assessment “excellent (9)” is given to a student who has displayed comprehensive, systematic knowledge of the educational program material, has independently performed all the tasks provided by the program, has deeply mastered the basic literature and is familiar with the additional literature recommended by the program, has been actively working in the classroom, has shown the systematic nature of knowledge on discipline sufficient for further study, as well as the ability to amplify it on one’s own, whose answer is distinguished by the accuracy of the terms used, and the presentation of the material in it is consistent and logical;

Assessment “excellent (8)” is given to a student who has displayed complete knowledge of the educational program material, does not allow significant inaccuracies in his answer, has independently performed all the tasks stipulated by the program, studied the basic literature recommended by the program, worked actively in the classroom, showed systematic character of his knowledge of the discipline, which is sufficient for further study, as well as the ability to amplify it on his own;

Assessment “good (7)” is given to a student who has displayed a sufficiently complete knowledge of the educational program material, does not allow significant inaccuracies in the answer, has independently performed all the tasks provided by the program, studied the basic literature recommended by the program, worked actively in the classroom, showed systematic character of his knowledge of the discipline, which is sufficient for further study, as well as the ability to amplify it on his own;

Assessment “good (6)” is given to a student who has displayed a sufficiently complete knowledge of the educational program material, does not allow significant inaccuracies in his answer, has independently carried out the main tasks stipulated by the program, studied the basic literature recommended by the program, showed systematic character of his knowledge of the discipline, which is sufficient for further study;

Assessment “good (5)” is given to a student who has displayed knowledge of the basic educational program material in the amount necessary for further study and future work in the profession, who while not being sufficiently active in the classroom, has nevertheless independently carried out the main tasks stipulated by the program, mastered the basic literature recommended by the program, made some errors in their implementation and in his answer during the test, but has the necessary knowledge for correcting these errors by himself;

Assessment “satisfactory (4)” is given to a student who has discovered knowledge of the basic educational program material in the amount necessary for further study and future work in the profession, who while not being sufficiently active in the classroom, has nevertheless independently carried out the main tasks stipulated by the program, learned the main literature but allowed some errors in their implementation and in his answer during the test, but has the necessary knowledge for correcting these errors under the guidance of a teacher;

Assessment “satisfactory (3)” is given to a student who has displayed knowledge of the basic educational program material in the amount necessary for further study and future work in the profession, not showed activity in the classroom, independently fulfilled the main tasks envisaged by the program, but allowed errors in their implementation and in the answer during the test, but possessing necessary knowledge for elimination under the guidance of the teacher of the most essential errors;

Assessment “unsatisfactory (2)” is given to a student who showed gaps in knowledge or lack of knowledge on a significant part of the basic educational program material, who has not performed independently the main tasks demanded by the program, made fundamental errors in the fulfillment of the tasks stipulated by the program, who is not able to continue his studies or start professional activities without additional training in the discipline in question;

Assessment “unsatisfactory (1)” is given to a student when there is no answer (refusal to answer), or when the submitted answer does not correspond at all to the essence of the questions contained in the task.

5. Methodological materials defining the procedures for the assessment of knowledge, skills, abilities and/or experience

The course is graded at an exam. The questioning starts with a random task assigned to each student and time given for completion of the task. No aids are allowed. The student then proceeds to a chat with the examiner, at which he/she presents his/her solution to the assigned task. The examiner then asks the student several questions that evenly cover the course content. A final grade is assigned based on the quality of answers and demonstrated level of understanding.