**CONTEMPORARY COMPUTATIONAL METHOD**

**1. GENERAL**

The course is focused on studying contemporary computational methods used in the theory of condensed states for model and first-principles research into ground state features, lattice, electronic and magnetic properties of metals, alloys, compounds, semiconductors and insulators. It includes the problems of calculating multi-electron systems, systems with strong correlations, static and dynamic approaches to implementing computational schemes in various bases. The objectives of the course are to study the principles, concepts and basic methods and approaches used in modern studies of the physics of the ground state of metals, alloys, semiconductors and insulators.

The work programme is based on:

* federal state, the requirements for the structure of the principal professional educational programme for postgraduate professional education approved by the order of the Ministry of Education and Science of the Russian Federation dated 16 March 2011 No 1365;
* Federal State Higher Educational Standard in the field of study 03.06.01 PHYSICS AND ASTRONOMY approved by the order of the Ministry of Education and Science of the Russian Federation dated 30 July 2014,
* the programme, qualifying examinations for the Ph.D. degree in the specialty 01.04.07 Condensed Matter Physics;
* the curriculum approved by the UrFU pro-rector.

As a result of mastering the discipline, a post-graduate student should:

**Know:**

* Equations of mathematical physics applied to the method of finite differences;
  + Physical models in calculations of the electronic structure of solids;
  + The augmented wave method and ways of constructing the muffin-tin potential.

**Be able:**

* + To determine the main characteristics of the phenomenon in question and the required accuracy of describing them. To evaluate the discarded parameters and characteristics;
  + To conduct the transformation of the Schrödinger equation into a homogeneous integral equation and implement its solution by the Green’s function method;
  + To build muffin-tin orbitals, and build wave functions and Bloch functions using muffin-tin orbitals.

**Master:**

* Instrumentation for the numerical solution of problems, computer systems and facilities based on UNIX systems;
* Hartree’s approach, the method of transforming the original Schrödinger equation into the system of integro-differential Hartree-Fock equations;
* The linearised augmented plane wave (LAPW) method and the technique of building the muffin-tin potential.

**2. STRUCTURE AND CONTENT OF THE WORK PROGRAMME**

2.1. **Learning session distribution** by semester

|  |  |  |  |
| --- | --- | --- | --- |
| Type of study | Number of hours (second year of study) | Work input | |
| Hour | Credit |
| Lectures | 18 | 18 | 0.5 |
| Practical exercises | - | - | - |
| Self-guided work | 90 | 90 | 2.5 |
| TOTAL | 108 | 108 | 3 |

**2.2. Contents of the discipline**

2.2.1. Topics, their content, volume in hours of lecture classes

|  |  |  |  |
| --- | --- | --- | --- |
| Number of subject | Subject content | Work input | |
| Hour | Credit |
| 1 | **1. Introduction. Equations of mathematical physics in the method of finite differences**  Statement and solution of the physical problem. Choice of approximations, an estimation of a degree of their severity. Determination of the main characteristics of the phenomenon under study and the required description accuracy. Evaluation of the discarded parameters and characteristics. Tools for solving problems numerically. Computing systems based on UNIX systems.  Basic types of differential equations. Interpretation and solution of the equations. Transition from differential equations to algebraic equations of the method of finite differences.  The method of finite differences and the scope of its application. The application of the apparatus of differential and integral calculus to continuum physics. The main idea of the finite difference method by the example of the stretched string dynamics analysis. Obtaining a system of finite-difference equations. The solution of an ordinary differential equation as an example of the application of difference schemes. The concept and criterion, the solution stability. | 4 |  |
| 2 | Quantum theory of multielectron systems and self-consistent field approximation. Physical models in calculations of the electronic structure of solids  Construction of the multielectron wave function. Slater’s determinant. Mean field approximation. Hartree’s approach. Transformation of the original Schrödinger equation into the system of integro-differential Hartree-Fock equations.  Pseudopotential methods. Model potentials. Slater potential, cellular potential, Hartree potential and Hartree-Fock potential. The transition from the multielectron problem to the single-electron one. Static model. Density functional method. Derivation of the density functional, Exchange-correlation potential. Slater approximation for the exchange-correlation potential. More accurate calculations of the total exchange-correlation potential. Calculation of excitation energies of the system. The physical meaning of the Lagrange multipliers. The transition state method.  Local density approximation (LDA). Basic equations L(S)DA. The class of problems solvable in the L(S)DA method. Accounting for electron-electron repulsion. Construction of the density functional taking into account electron-electron correlations at the node. Static mean field approximation. The basic equations are LSDA + U. The class of problems solvable in the L(S)DA + U method. Motov insulators. Charge and orbital ordering Description of the Mott-Hubbord metal-insulator transitions.  Generalisation of the L(S)DA + U method to systems with the strong spin-orbit interaction. The basic equations are L(S)DA + U + SO. The class of problems solvable in the L(S)DA + U + SO method. | 4 |  |
| 3 | Orthogonalised plane waves and pseudopotential. Strong communication method  Wave functions of valence states of an atom. Determination of orthogonalised plane waves (OPW). The basis of OPW. OPW overlapping. Decomposition of Bloch functions on the basis of OPW. Pseudopotential on the basis of OPW. Heine-Abarenkov pseudopotential. The secular equation on the OPW basis and its solution. Disadvantages of the OPW method.  The basis of atomic orbitals. Connection of Bloch functions and atomic orbitals. Construction of molecular orbitals. Derivation and solution of the secular equation on the basis of atomic orbitals. Matrix overlap elements. | 4 |  |
| 4 | Augmented wave method and the construction of the muffin-tin potential. KKR method in the muffin-tin potential approximation.  Muffin-tin approximation for the intra- and interatomic regions. The augmented wave as a result of cross-linking the Schrödinger equation solutions in the intra- and interatomic region. Complete Blokhov’s. function. Derivation and solution of the secular equation on the basis of the augmented waves. The rate of convergence of the method.  Transformation of the Schrödinger equation into a homogeneous integral equation and its solution by the Green’s function method. The formulation of the Korringa–Kohn–Rostoker method (KKR). Expansion of the Green’s function with respect to spherical harmonics. Structural constants of the KKR method. Representation of the KKR equations through phase shifts of scattering by a muffin-tin potential. Practical aspects of the KKR method implementation. The rate of its convergence. | 4 |  |
| 5 | Linearised methods. Determination of the density of states and the construction of energy bands.  Approximation of atomic spheres and secular equation. Anderson approximation for the volume approximation in the overlapping sphere scheme. Construction of muffin-tin orbitals. Construction of wave functions and Bloch functions using muffin-tin orbitals. Linearisation of muffin-tin orbitals. The linearized augmented plane wave (LAPW) method and construction of the muffin-tin potential. Construction of the basis and formulation of the LMTO method. Getting a secular equation and its solution. Definition of overlap matrices. Orthogonalisation of LMTO Basis and formulation of the orthogonalised LMTO method of. The secular equation and its solution. Comparison of the rate of convergence of linearised methods.  Density of states and integration in inverse space by the tetrahedron method. Construction of surfaces of equal energies in the Brillouin zone. Obtaining a formula for calculating the density of a state. Linearization of energy inside the tetrahedron. Differential and integral density of states. | 2 |  |
|  | TOTAL | **18** | **0.5** |

**2.2.2. Practical exercises, their content, volume in hours.**

Practical classes in this discipline are not applicable.

**2.2.3. Self-guided work of post-graduate students**

|  |  |  |  |
| --- | --- | --- | --- |
| Subjects of the self-study work programme | List of tasks for the self-guided work | Work input | |
| Hour | Credit |
| Equations of mathematical physics in the method of finite differences | Analysis of the scientific and technical literature and electronic sources taking into account the content of the discipline | 20 |  |
| Quantum theory of many-electron systems and approximation of a self-consistent field. Physical models in calculations of the electronic structure of solids | Analysis of the scientific and technical literature and electronic sources taking into account the content of the discipline | 20 |  |
| Orthogonalised plane waves and pseudopotential. Strong communication method | Analysis of the scientific and technical literature and electronic sources taking into account the content of the discipline. Completing computational tasks | 20 |  |
| The method augmented waves and the construction of the muffin-tin potential. KKR method in the muffin-tin potential approximation. | Analysis of the scientific and technical literature and electronic sources taking into account the content of the discipline. Completing computational tasks | 20 |  |
| Linearized methods. Determination of the density of states and the construction of energy bands. | Analysis of the scientific and technical literature and electronic sources taking into account the content of the discipline. Completing computational tasks | 10 |  |
|  | **ИТОГО** | **90** | **2.5** |

**References**

* S. Cottenier, Density Functional Theory and the family of (L)APW-methods: a step-by-step. introduction (Instituut voor Kern- en Stralingsfysica. K.U.Leuven, Belgium), 2008, ISBN 90-807215-1-4 (to be found at http://www.wien2k.at/reg user/textbooks).
* D. Singh. Planewaves, pseudopotentials and the LAPW-method, Kluwfer Academic Publishing (1994), ISBN 0-7923-9421-7.

**2.3.2 List of test questions for preparation for the final certification of the discipline**

1. Problems of describing a multielectron atom. Correlated state. The method of finite differences and the scope of its application.
2. Application of the apparatus of differential and integral calculus to continuum physics.
3. The basic idea of the method of finite differences based on the example of the tension string dynamics analysis. The concept and criterion, the stability of the solution.
4. Construction of the multielectron wave function.
5. Necessity and methods for building a model potential.
6. Mean field approximation. The Hartree and Hartree-Fock approach.
7. Pseudopotential methods. Effective potential of the environment. Model potentials. Slater potential. cellular potential, Hartree potential and the Hartree-Fock potential.
8. Density functional method. Derivation of the density functional.
9. Exchange - correlation potential.
10. Calculation of the system excitation energies. The physical meaning of the La Grange multipliers. The transition state method. Local density approximation.
11. Basic LDA + U equations. The class of problems solvable in the LDA + U method. Mott insulators. Charge and orbital ordering. Description of the Mott-Hubbord metal-insulator transitions.
12. Approximation of the dynamic mean field (DMFT). Basic DMFT equations and their solution.
13. Quantum Monte Carlo method. Hirsch-Fai solution.
14. Quantum Monte Carlo method with continuous time CT-QMK
15. Solution of the radial equation and the equation for the angular part of the Schrödinger equation. The Numerov method for the numerical solution of second-order differential equations.
16. Definition of the structural factor.
17. Construction of energy zones. and the secular equation for the energy bands. Approximation of free electrons and flat
18. Valent levels. Wave functions of valence states of an atom.
19. The basis of OPW. OPW overlapping. Decomposition of Bloch functions in the OPW basis, Heine-Abarenkov pseudopotential. The secular equation on the OPW basis and its solution.
20. Construction of molecular orbitals. Derivation and solution of the secular equation on the basis of atomic orbitals. Matrix overlap elements.
21. ‘Muffin-tin’ approximation for the intra- and inter-atom areas.
22. The augmented wave as a result of cross-linking the solutions of the Schrödinger equation
23. The formulation of the Korringa-Kohn-Rostoker method (KKR).
24. Expansion of the Green's function with respect to spherical harmonics. Structural constants of the KKR method.
25. Practical aspects of the KKR method implementation. Rate of convergence.
26. Approximation of atomic spheres and secular equation. Anderson approximation. Construction of muffin-tin orbitals.
27. Linearisation of muffin-tin orbitals.
28. Construction of the basis and formulation of the LMTO method. Definition of overlap matrices, LMTO orthogonalisation. Construction of a basis. Method of the orthogonalised LMTO.
29. Density of states and integration in inverse space by the tetrahedron method. Construction of surfaces of equal energies in the Brillouin zone.
30. Differential and integral density of states