Annex 1.

Form of opening (renewal) for Theme /
Large Research Infrastructure Project

APPROVED

JINR Vice-Director

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THEME PROPOSAL FORM

Opening/renewal of a theme/large research infrastructure project within the Topical plan of JINR

1. General information on the theme / large research infrastructure project (hereinafter LRIP)

1.1. Theme code / LRIP (for extended themes) – ***01-3-1137-2019/2023***

1.2. Laboratory **Bogoliubov Laboratory of Theoretical Physics**

1.3. Scientific field **Theoretical Physics**

1.4. The title of the Theme / LRIP **Theory of Complex Systems and Advanced Materials**

1.5. Theme / LRIP Leader(s) **V.A. Osipov and A.M. Povolotsky**

1.6. Theme / LRIP Deputy Leader(s)

2. Scientific case and theme organization

2.1. Annotation

The most important directions of fundamental research will be theoretical studies of physical phenomena and processes in condensed matter, studies of properties of new advanced materials, constructing and analysis of theoretical models and development of analytical and computational methods for their solution. Complex materials, such as high-temperature superconductors, magnetic materials, smart composite materials, fractal and layered structures are supposed to be studied and a wide class of systems with strong electronic correlations will be analyzed. Theoretical research in this area will be aimed at supporting the experimental study of these materials, carried out at the Frank Laboratory of Neutron Physics, JINR. It is planned to conduct research in the field of physics of nanostructures and nanomaterials, in particular using the software packages for modeling physical and chemical processes and for analysis of physical characteristics. First of all, these are modern two-dimensional materials, such as graphene, transition metal dichalcogenides, etc., including their modification and chemical functionalization for subsequent use in the design of new devices for nanoelectronics, spintronics, etc. Partly, these studies are focused on experiments held at the FLNR Center for Applied Physics JINR, the Institute of Semiconductor Physics SB RAS and a number of other laboratories of the JINR Member States. The physical properties of stacks of Josephson junctions and various Josephson nanostructures will be studied in detail. Much attention will be paid to the analysis of both lattice and field models of equilibrium and nonequilibrium systems of statistical mechanics. The concepts of scaling and universality allow one to go beyond the model approach and to apply the results obtained to broad classes of phenomena studied in the physics of condensed matter. Studies of a wide range of universal phenomena in complex systems - phase transitions in condensed matter and high-energy physics, scaling in (magneto)hydrodynamic turbulence, chemical reactions, percolation, etc. by the methods of quantum field theory including the functional renormalization group are supposed to be carried out.

2.2. Projects in the Theme / LRIP subprojects

Project 1: Complex materials (project leader **E. M. Anitas)**

Project 2: Mathematical models of statistical physics of complex systems (project leader **A.M. Povolotsky)**

Project 3: Nanostructures and nanomaterials (project leaders **V.A. Osipov, E.A. Kochetov)**

Project 4: Methods of quantum field theory in complex systems (project leader **Michal Hnatic)**

2.3. Scientific case (no more than 20 pages)

(aim, relevance and scientific novelty, methods and approaches, techniques, expected results, risks).

The main objectives of the research will be:

- theoretical studies of physical phenomena and processes in condensed matter, studies of properties of new advanced materials, constructing and analysis of theoretical models and development of analytical and computational methods for their solution.
- The construction and studies of mathematical models of statistical physics of complex systems and related models of quantum mechanics and quantum field theory with an emphasis on the concepts and structures of the theory of integrable systems as well as the development of mathematical tools lying at the core of this theory, including the theory of special functions and representation theory of quantum matrix algebras and braid groups.
- Investigations of the properties of new promising materials, primarily nanostructures and nanomaterials. Particular attention will be paid to the analysis of the transport characteristics of two-dimensional and few-layer structures, taking into account their functionalization and structural modification. An important place will be occupied by the study of such phenomena as topological superconductivity in strongly correlated systems and the manifestation of the Josephson effect in hybrid heterostructures. This is explained not only by the fundamental nature of the physical properties of these materials, but also by their practical importance for designing new electronic devices, as well as devices for storing, processing and transmitting information, sensors and biosensors, and others.
- Studies of stochastic nonlinear dynamic systems, such as developed (magneto)hydrodynamic turbulence, nonequilibrium phase transitions, phase transitions in systems with high spins, kinetics of chemical reactions, percolation processes, surface growth in random media and self-organized criticality.

Relevant complex materials that are aimed to be investigated are atomically thin semiconductors colossal magneto-resistance compounds, heavy-fermion systems, low-dimensional quantum magnets with strong spin-orbit interaction or topological insulators. They attract now considerable attention, both from the point of view of fundamental studies and as promising materials for applications, e.g., the quantum computing, will be analyzed. Similarly, smart composite materials, fractal and layered structures, and biological macromolecules will be also analyzed.

Recently, a significant progress has been made in understanding the nature of limit shapes, universal fluctuations and correlations in models of equilibrium and non-equilibrium statistical physics. Among the equilibrium models the dimer packings and polymers on lattices, polymers in random media, vertex and spin models are studied, where the subject of study is, for example, the limiting macroscopic shape of the boundaries between different thermodynamic phases, as well as its random fluctuations and correlations between its parts. In the nonequilibrium context, similar issues are studied on the basis of particular stochastic models of nonequilibrium lattice gases or traffic flows like the asymmetric simple exclusion process, as well as various interfaces moving under the action of random forces, where the macroscopic description is given in terms of solutions of hydrodynamic type equations and random fluctuations characterized by the universal statistical laws specific for vast universality classes unifying a number of natural phenomena, like e.g. the prominent Kardar-Parisi-Zhang universality class.

The advances made in these directions were due to novel applications of the theory of integrable systems to derivation of exact results in various models with many degrees of freedom. Using concepts of universality and scaling these results can often be extended to a whole universality class of natural phenomena. The progress became possible due to construction of new integrable models of non-equilibrium stochastic systems, systems of equilibrium statistical physics and quantum systems, development of new methods of exact solutions of these models and discovery of new mathematical structures standing behind the integrability, like new classes of special functions and new solutions of the Yang-Baxter equations and braid relations appearing in the representation theory of quantum matrix algebras and braid groups. Many cutting-edge results in these directions were obtained by the team involved in this project.

At this stage, the development of electronics has reached a limit, which is primarily due to the properties of the material basis of microelectronic devices, that is, due to the properties of standard semiconductors. In this regard, there is a request to fundamental science regarding the further development of the base for computing technology. One of the answers is the proposal of the fundamentally new materials with unique properties and the development of the ways to use of them to create new efficient microelectronic devices. Graphene is one of the main candidates for the role of a basic material for a new type of electronics owing to a number of advantages over standard semiconductors. The most important is the extremely high mobility of charge carriers (this characteristic is directly responsible for performance of electronic devices). In addition, the very fact that graphene is two-dimensional (2D) creates the possibility for a compact layout (miniaturization). However, this material also has some disadvantages. If we omit the technological aspects, then they should include the absence of a band gap and the inability to localize electrons in graphene due to the Klein paradox. The development of fundamental principles for the operation of electronic devices, which, on the one hand, use the advantages of graphene, and on the other hand, allow avoiding the difficulties associated with its shortcomings, is an extremely urgent and very interesting scientific task.

Recent years have seen a surge in superconducting quantum electronics, with rapidly rising number of promising devices and systems enabling quantum coherent manipulation. Topological order in strongly correlated systems, including quantum spin liquids, quantum Hall states in lattices and topological superconductivity is one of the key topics. Various metallic non-Fermi-liquid states including fractionalized Fermi-liquid and phase string theories are being intensively researched. Classification of topological states and differences between quantum and classical topology are of particular interest. Along with important practical applications the new topological paradigm may contribute to our understanding of fundamental questions of nature.

The Josephson effect finds numerous applications in various fields of science, technology, and medicine. In particular, devices based on it are used in superconducting electronics for measuring ultra-weak magnetic fields, in quantum metrology as modern voltage standards, and in medicine for recording magnetoencephalograms of the brain. This effect is the basis for generating and detecting coherent electromagnetic radiation in the terahertz region. Until recently, it was not possible to combine superconductivity and magnetism, since these phenomena are antagonistic: a magnetic field destroys superconductivity, and superconductivity pushes out a magnetic field. However, in hybrid Josephson structures they have been brought close enough to allow superconductivity to control magnetism and magnetism to influence superconductivity. One of the main directions in this area is the solution of fundamental problems of superconducting spintronics - the development of fundamentally new methods for controlling the magnetization of magnets, as well as a radical reduction in energy consumption during the operation of spintronic devices.

Dynamic nonlinear systems in which nonequilibrium (stochastic) fluctuations of physical quantities is one of the most important research topics by leading scientific teams in the world. They cover a wide range phenomena that we observe in the world around us. Stochasticity is a fundamental property of physical, chemical, biological and even socio-economic phenomena.

Notable examples of stochastic processes include - hydrodynamic and magnetohydrodynamic turbulence, describing, in particular, turbulent movements in the Earth's atmosphere and oceans, the spread of pollutants in them substances (including chemically active), as well as chaotic motions of plasma on surface of the sun and in space. One of the important consequences of the existence of mechanical instabilities in electrically conducting turbulent media is an exponential growth of magnetic fluctuations leading to the formation of observed nonzero averaged magnetic fields only due to the kinetic energy of the turbulent medium.

Another important example of stochastic systems are percolation processes. They describe phenomena such as seepage in porous media, filtration, spread of infectious diseases, forest fires and others. Their universal feature is the existence of a nonequilibrium phase transition to an inactive (absorbing) state that extinguishes all activity of the observed system.

Obviously, the study of transitions between a stationary active (which does not correspond to thermal equilibrium) and the inactive phase is of great practical importance. Note that these transitions are continuous and are especially interesting as prototypical examples of strongly non-equilibrium critical behavior.

The main object of study are physical quantities that depend on space-time coordinates and therefore are fluctuating fields, and the measured quantities are their statistical averages. The most important of them are non-zero average field values, response functions, multipoint correlation functions, two-point simultaneous correlations (structural functions), including composite fields (operators). In the region of large spatial and temporal scales, their scaling behavior with universal critical exponents is observed. The analysis of stability regions of scaling regimes and the calculation of indices is a priority goal in the study of stochastic nonlinear systems.

The **relevance and scientific novelty** of the planned results

- lies in the analysis of a wide range of physical characteristics of new materials in order to identify the most promising for the development and creation of devices in the field of nanoelectronics, spintronics, photonics, etc.
- follow the modern trends in exact solutions of systems with many degrees of freedom and are based on rich background of the team in the theory of integrable systems and its applications as well as in theory of special functions and theory of quantum groups.
- is found in the study of scaling regimes, which includes the calculation of critical exponents and representative physical constants and parameters of the systems under consideration in higher orders of perturbation theory.

General **methods** of theoretical research and approaches to solving the formulated problems are based on the use and improvement of the methods of quantum solid state physics, physical kinetics, quantum mechanics and quantum chemistry, quantum field theory, equilibrium and nonequilibrium statistical physics. Numerical methods, as well as the use of standard software packages for quantum chemical calculations, Ab initio calculations, molecular dynamics simulations, etc will be used. Existing methods in the theory of integrable systems like the coordinate algebraic and functional Bethe ansatz, quantum inverse scattering method, methods of functional relations and the theory of finite-difference equations, methods of integrable probability like the theory of determinantal and Pfaffian point processes, Markov dualities, etc. will be extended and generalized. The theory of renormalizations, calculations of multi-loop Feynman diagrams, algorithms for resumming the terms of a perturbation theory series with respect to a formally small parameter, the technique of the renormalization group, the functional renormalization group, methods for solving equations like the Langevin equation and its generalizations, the Fokker-Planck equation, master equations for distribution functions, high-performance computations, including computations on a supercomputer are planned to be used.

The specific goals and objectives of the project are as follows**:**

- Establishing a semi-analytical relationship between the energy and size of the excitons in atomically thin semiconductors and the average dielectric constant to its immediate dielectric surroundings. Deriving the long-range dipole-dipole interaction between excitons in their excited states

- Theoretical and experimental investigations of the structure of complex hierarchical systems, including fractals and biological macromolecules.

- Estimation of the exchange parameters of Kitaev materials based on transition and rare-earth metals and calculation of their spin-wave spectrum.

- Theoretical investigations of electronic properties of nanoparticles for electronics research.

- Theoretical and experimental investigations of dense random packing with a power-law size distribution at nano and micro scales.

- Application and development of quantum algorithms for computational problems in condensed matter physics and quantum chemistry.

- Development of a theory of stability for mixtures of quantum fluids.

- Numerical and experimental investigation of irradiation resistance of various compounds.

- Study of various reaction-diffusion models of interacting particles on one-dimensional lattice with the use of Markov dualities. Construction and full exact solution of new stochastic models describing statistics of lattice paths or particles with discrete time dynamics, which allows one to incorporate new types of interaction compared to the continuous time models studied earlier.

- The calculation of exact cluster densities and their asymptotic expansions in the bond percolation, as well as densities of loops in the related densely packed loop models on the lattices with different boundary conditions, which is possible due to a connection of these problems with the Bethe ansatz solvable six-vertex model, construction of asymptotic expansions of thermodynamic quantities characterizing finite-size behavior of the free fermionic lattice models, such as dimers, Ising and spanning trees with different geometries under different boundary conditions. Study of the boundary behavior of nonlocal correlations in dense polymer and spanning tree models and characterization of the limit shapes and universal fluctuations of polymer configurations.

- Applications of the studied polymer models and quantum spin chains to problems from adjacent areas of quantum mechanics and biophysics. Studies of «entangled states» and magnetic properties of complex quantum spin systems relevant for quantum computing problems. Applications of the rotor-router (Eulerian walk) model to studies of the dynamics of double-stranded DNA breaks.

- Development of mathematical structures standing behind the integrability. In particular, the elliptic beta-integrals and elliptic hypergeometric functions, which were discovered at BLTP and form the top-level special functions of mathematical physics comprising most of known special functions as particular limiting cases, provide the most profound mathematical framework for the theory of integrable systems. The research planned under the project includes further investigation of the properties of these functions and of their various limiting forms. In particular, this is the search for applications of these functions in quantum field theory, quantum and statistical mechanics, and in the theory of solitons. There are plans to generalize obtained results to the cases of rarefied hypergeometric functions of various types and to describe the relevant physical systems, as well as to investigate connections between soliton solutions of integrable equations, lattice Coulomb gases, non-local Ising chains and ensembles of random matrices.

- Studies of algebraic structures behind the integrability and their use for constructing new integrable systems which could be useful in various applications. In particular, investigations of a family of quantum matrix algebras will be continued. These algebras were discovered in the context of the quantum inverse scattering method and have found various applications in the theory of integrable systems, quantum mechanics and field theory, statistical physics and the theory of stochastic processes.

- In order to identify materials with promising properties for use as a component base for a new generation of electronics, it is planned to study thermal and electron transport in low-dimensional materials of various configurations and chemical composition. An analysis will be made of the role of functionalization, structural modification, the influence of thin layers, polycrystalline, structural defects, and other factors. Experimental studies are carried out in cooperation with the Institute of Semiconductor Physics SB RAS (synthesis, characterization, functionalization) and FLNR JINR (ion irradiation to create nanopores).

- Analysis of topological superconductivity in strongly correlated electronic systems in order to search for possible applications for the transmission and storage of quantum information and for the study of non-standard quantum transport, insensitive to local noise sources.

- Study of dynamic, transport and chaotic phenomena in hybrid Josephson nanostructures with magnetic materials for the purposes of superconducting spintronics. Modeling of quantum phenomena in Josephson qubits (memory elements).
- Study of the properties of polarons in low-dimensional materials and nanostructured objects. Analysis of plasmon-phonon interaction and plasmons in nanoscale and massive objects.

- Investigation within the BEC-BCS functional renormalization group of the crossover in systems of multicomponent fermions: analysis of phase diagrams and calculation of transition temperatures to the ordered state. Approbation and adaptation of computational methods for solving nonperturbative equations of the functional renormalization group.

- Development of computational methods for calculating the contributions of multiloop diagrams to the renormalization group functions of dynamical models. Investigation of the dynamics of the superconducting phase transition in low-temperature superconductors.

- Study of the effects associated with the violation of mirror symmetry in magnetohydrodynamic developed turbulence. Calculation of two-loop Feynman diagrams generated by the Lorentz force and two-loop diagrams of the response function leading to an exponential growth of magnetic field fluctuations in the region of large scales. Study of the phenomenon of turbulent dynamo.

- Construction of effective field-theoretical models of chemical reactions of various types of particles occurring in random media. Study of infrared scaling behavior of statistical correlations of particle densities by renormalization group methods.

- Study of isotropic and directed percolation. Calculation of multiloop Feynman diagrams generating ultraviolet divergences. Finding fixed points of the renormalization group equations and calculating critical exponents for physically significant and experimentally observable quantities - response functions, density of active nodes (agents), effective radius and mass of active zones.

- Study of the effect of isotropic motion of a medium with different statistical characteristics on the possibility of anisotropic scaling in the Hua-Kardara self-organized criticality model. Investigation by the functional renormalization group method of possible asymptotic regimes corresponding to the non-universal scaling behavior of a surface growing in a random environment and described by a model that includes an infinite number of types of interactions.

Both employees of JINR laboratories and representatives of scientific institutions and universities of Russia, the JINR Member States and a number of other countries are involved in solving the problems of the project.

2.4. Participating JINR laboratories

- Frank Laboratory of Neutron Physics (A.S. Doroshkevich, A.I. Kuklin).
- Meshcheryakov Laboratory of Information Technology (Z.A. Sharipov, Z.K. Tukhliev, E.P. Yukalova, P.V. Zrelov, O.V. Ivancova, L.A. Siurakshina, J. Busa, I. Sarhadov, S.I. Serdyukova, E.B. Zemlianaya).
- Flerov Laboratory of Nuclear Reactions (M. N. Mirzayev, V.A. Skuratov).
- Dzhelepov Laboratory of Nuclear Problems (E. P. Popov).
- Laboratory of Radiation Biology (A.N. Bugay).

2.5. Participating countries, scientific and educational organisations:

Organization	Country	City	Participants	Type of agreement
Institute of Solid State Physics	Bulgaria	Sofia	H. Chamati	Joint work
University of Sao	Brazil	Sao Carlos	V. S. Bagnato	Joint papers

Paulo				
West University of Timisoara	Romania	Timisoara	I. Bica	Joint work
NRU HSE	Russia	Moscow	Gritsenko V.A.	Exchange of visits
NRU HSE	Russia	Moscow	Krotkov D.I.	Joint works
NRU HSE	Russia	Moscow	Uvarov F.V.	Exchange of visits
NRU HSE	Russia	Moscow	Gorbunov V.G.	Exchange of visits
NRU HSE	Russia	Moscow	Khoroshkin S.M.	Exchange of visits
SPDMI RAS	Russia	St. Petersburg	Derkachev S.E.	Joint works
SPDMI RAS	Russia	St. Petersburg	Mudrov A.I.	Exchange of visits
SPDMI RAS	Russia	St. Petersburg	Bytsko A.G.	Exchange of visits
IHEP	Russia	Protvino	Sapronov P.A.	Joint works
IHEP	Russia	Protvino	Razumov A.V.	Exchange of visits
YerPhI	Armenia	Yerevan	Apresyan E.	Joint works
YerPhI	Armenia	Yerevan	Izmailyan N.S.	Joint works
YerPhI	Armenia	Yerevan	Ananikyan N.S.	Joint works
YSU	Armenia	Yerevan	Morozov V.F.	Joint works
YSU	Armenia	Yerevan	Mamasakhlisov E.S.	Joint works
Institute of Mechanics BAS	Bulgaria	Sophia	Bnzarova N.	Joint works
Institute of Mechanics BAS	Bulgaria	Sophia	Pesheva N.	Joint works
UdeM Mathematical Research Center	Canada	Montreal	Loutsenko I.M.,	Joint works
Caltech	USA	Pasadena		
University of Wuppertal	Germany	Wuppertal	Rains E.M.	Joint works
Aix-Marseille University	France	Marcel		Exchange of visits
Angers University	France	Angers	Boos G.	Joint works
University of Warwick	Great Britain	Warwick	Ogievetsky O.	Exchange of visits
University of Sydney	Australia	Sydney	Rubtsov V.	Joint works
NAU	Australia	Canberra	Zaboronsky O.	Exchange of visits
IP NASB	Belarus	Minsk	Kilin S.Ya. +5	visits
SPMRC NASB	Belarus	Minsk	Saiko A.P. +3	visits
IIP UFRN	Brazil	Natal, RN	Ferraz A.	joint work
CU	Egypt	Giza	El Sherbini T.M.	joint work
IACS	India	Kolkata	Sengupta K.	joint work
IASBS	Iran	Zanjan	Kolahchi M.	joint work
IPT MAS	Mongolia	Ulaanbaatar	Sangaa D.	visits
WUT	Poland	Wroclaw	Mierzejewski M.	joint work

NIIC SB RAS	Russia	Novosibirsk	Okotrub A.V. +3	visits
ISP SB RAS	Russia	Novosibirsk	Antonova I.V.+2	visits
SSU	Russia	Saratov	Kolesnikova A.S.	joint work
UB	Romania	Bucharest	Nemnes G.A.	joint work
INS “VINCA”	Serbia	Belgrade	Tekic D.	joint work
CU	Slovakia	Bratislava	Plecenik A.	joint work
IEP SAS	Slovakia	Kosice	Pudlak M. +1	visits
UNISA	South Africa	Pretoria	Bota A.E.	joint work
UU	Japan	Utsunomiya	Irie A.	joint work
SPSU	Russia	Sankt Petersburg	Gulitsky N. + 2	common publications
RUDN	Russia	Moscow	Kulyabov D. + 2	common publications
P J Šafarik University	Slovakia	Košice	Lucivjansky + 2	common publications
Helsinki University	Finland	Helsinki	Honkonen J.	common publications
Leipzig University	Germany	Leipzig	Bordag M.	common publications
IM BAS	Belarus	Minsk	Malyutin V.	common publications

2.6. Key partners *(those collaborators whose financial, infrastructural participation is substantial for the implementation of the research program on the theme. Example – JINR participation in the LHC experiments at CERN).*

3. Manpower
3.1. Manpower needs in the first year of implementation

No.	**Personnel category**	**JINR staff, FTE amount**	**JINR associated personnel, FTE amount**
1.	research scientists	**45/40**	
2.	engineers		
3.	specialists		
	Total:	**45/40**	

3.2. Available manpower
3.2.1. JINR staff (total number of participants)

No.	**Personnel category**	**Division**	**Position**	**Amount FTE**
1.	research scientists	SDTCM	**40**	**35.1**

2.	engineers			
3.	specialists			
	Total:		**40**	**35.1**

3.2.2. JINR associated personnel

No.	**Personnel category**	**Partner organization**	**Amount of FTE**
1.	research scientists		
2.	engineers		
	Total:		

4. Financing
4.1. Total estimated cost of the theme / LRIP

No.	**Items of expenditure**	**Cost**	**Expenditure per year (thousands of the US dollars)**						
			1st year	2nd year	3rd year	4th year	5th year	6tht year	7th year
1.	International cooperation	542,0	65,8	70,8	74,9	77,9	81,0	84,1	87,5
2.	Materials								
3.	Equipment, Third-party company services								
4.	Commissioning								
5.	R&D contracts with other research organizations								
6.	Software purchasing								
7.	Design/construction								
8.	Service costs (*planned in case of direct affiliation)*								
TOTAL:		**542,0**							

4.2. Extra funding sources

Expected extra funding from partners/customers (total for all projects).

AGREED:

Chief Scientific Secretary

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Laboratory Director

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"_____"__________________202_г.

Head of BEPD
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"_____"__________________202_г.

Head of DSOA
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Head of HRRMD
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Scientific Secretary of the Laboratory
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Laboratory Economist
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Theme leader
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