Form № 21

APPROVED BY JINR Vice Director

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SCIENTIFIC AND TECHNICAL JUSTIFICATION FOR OPENING A NEW THEME OR FOR EXTENDING THEME to be included in the TOPICAL PLAN FOR JINR RESEARCH FOR 20<u>19</u>–20<u>23</u>

 Theme code
 Laboratory
 BLTP

 Department
 SD CMT

 Research area
 Theoretical physics

 Theme title
 Theory of Complex Systems and Advanced Materials

 Theme leaders
 V.A. Osipov, A.M. Povolotsky

Abstract

The scientific program of research for 2019-2023 in the framework of the theme "Theory of complex systems and advanced materials" of BLTP assumes the further development of analytical and numerical methods for studying complex many-body systems that are of current interest in modern condensed matter physics, the development of mathematical models of such systems and the identification of universal laws on an example of studied models. A particular attention will be paid to both lattice and field-theory models of equilibrium and non-equilibrium statistical systems and to modeling a wide class of new materials, including nanostructured materials, which are of great practical importance. The concepts of scaling and universality allow us to go beyond the model approach and to apply the results obtained to broad classes of phenomena studied in the physics of condensed matter at JINR. It is important to note the markedly growing interdisciplinary nature of research, where condensed matter physics and statistical physics, closely intersect with atomic and nuclear physics, particle physics, mathematical physics, astrophysics, and biology. Below, in a structured form, the planned main topics of theoretical research are presented in the framework of the stated theme.

Experimental studies directly point to an important relationship between the structural and physical properties of materials. In particular, correlations between magnetism and structural properties of heavy rare-earth metals at high pressures are observed. A combined theoretical and experimental study of effects of high pressure on the structural, electronic and magnetic properties of heavy rare-earth metals is planned. Changes of the lattice and magnetic structural properties under an applied

pressure will be measured at the Laboratory of Neutron Physics, JINR. The measured data will be interpreted with the use of both the model analysis and the *ab initio* band structure calculations based on methods of density-functional theory at the Laboratory of Theoretical Physics, JINR.

Pronounced correlations between the physical properties of various fractal systems and their geometrical structure at nano and micro scales have been observed. Theoretical and experimental investigations of the structure of complex hierarchical systems, including surface fractals and multifractals, will be performed for the purpose of explaining physical characteristics of nanomaterials with applications to modern nanotechnologies. Experimental methods are based on small-angle scattering of neutrons, which is relevant to the use of IBR-2 pulsed reactor at LNP JINR, as well as x-rays and/or light scattering.

Investigation of electronic properties, collective excitations (charge density waves, spin waves), phase transitions in complex systems such as strongly-correlated electronic systems, low-dimensional quantum magnets with complicated lattice is one of the most important problems in condensed matter physics. These studies will be performed on the basis of the nonperturbative methods of Green functions developed in BLTP JINR. The results obtained will be used to explain the experimental results found in investigations of copper-oxide compounds and two-dimensional electronic systems with the graphene-like structure.

Cuprate high-temperature superconductors belong to one of the most intricate strongly correlated electron systems. The theoretical analysis of such systems is challenging, because the traditional methods like the perturbation theory and the adiabatic continuation fail. It is planned to apply tools based on the quantum Monte Carlo method, which were developed in the BLTP, to study the properties of the superconducting phase in cuprates. This will allow a description of the structure of the Fermi surface in doped cuprates explaining possible mechanisms of high-temperature superconductivity.

It is planned to develop theoretical description of equilibium and nonequilibrium properties of finite quantum systems, including trapped atoms and molecules, dipolar and spinor nanosystems, and complex quantum networks. The main purpose is to investigate the possibility for regulating the properties of such finite quantum systems for quantum information processing. The following theoretical methods, developed in BLTP JINR will be used: scale separation approach, self-consistent theory of strongly correlated systems with spontaneous symmetry breaking, self-similar approximation theory. Also, numerical calculations will be employed.

One of the main topics of modern condensed matter physics is the study of nanostructures and nanomaterials. This is not only due to the fundamental nature of their physical properties, but also owing to the practical importance for the creation of new electronic devices, storage devices, processing and transmission of information, sensors and biosensors, and others.

A special role is played by the two-dimensional materials: graphene, phosphorene, silicene, and others. Theoretical investigations of the influence of localized boundary states in various twodimensional materials on electronic transport are planned. In particular, effects such as electronphonon interaction, the role of the substrate and external electromagnetic radiation will be taken into account. A theoretical study of thermal and electronic transport in polycrystalline two-dimensional structures is also planned. It will help to improve the quality of modern thermoelectric materials. In addition, the effect of structural defects on the kinetic properties of new materials will be investigated.

The two-dimensional materials are actively used as elements for developing highly sensitive sensors for various objects detection: from toxic metals and gases to complex biomolecules and even bacteria. A particular attention is paid to the sensors based on graphene because of their unique physical properties: attachment of biological molecules (proteins, DNA, RNA) to graphene increases

the selectivity and sensitivity of the sensor, which opens up wide possibilities for using such devices as express analyzers in medical research. It is planned to study the transport properties of systems formed by low-dimensional structures with detector biomolecules attached to them, in order to analyze the sensory characteristics of these devices. The quantum electrodynamic and correlation effects in atomic systems in nanostructured and biological materials will be studied for the description of the processes of transmission and processing of quantum information.

The functionalization of new nanomaterials plays an important role. A detailed theoretical analysis of the physical properties of fluorinated and oxidized graphene is planned. Experimental studies are carried out in cooperation between the Institute of Semiconductor Physics of the SB RAS (synthesis, characterization) and the FLNR of JINR (ion irradiation for the creation of nanopores).

Investigation of resonance, chaotic and topological features of Josephson nanostructures and superconducting devices is planned. Dynamics and current-voltage characteristics of superconductor-ferromagnet-superconductor structures for superconducting spintronics will be studied.

The solution of many stated problems relies on computer modeling within the framework of packages for quantum chemical calculations, molecular dynamics and density functional. For this reason, it is planned to work closely with LIT JINR, first of all, by using the supercomputer "Govorun".

Last years a significant advance in understanding of limit shapes, universal fluctuations and correlations in models of equilibrium and non-equilibrium statistical physics was achieved. Among the equilibrium models being studied are the dimer packings, lattice polymers, polymers in random media, vertex and spin lattice models, where the subject of studies is, for example, a limit macroscopic shape of interfaces between different thermodynamic phases as well as their random fluctuations and correlations between them. In the non-equilibrium context similar questions are addressed to stochastic models of non-equilibrium lattice gases or traffic flows as well as to models of interfaces growth subject to a random force, where the macroscopic description is given in terms of hydrodynamic-like equation, while the random fluctuations reveal the universal properties.

The studies of statistics of particle flows on the lattices in stochastic models like exclusion processes with generalized interactions, zero-range processes and avalanche processes are planned. Their evolutions are also tightly connected with the evolution of interfaces subject to random forces. The universal fluctuations and correlations of particle flows in these models will be characterized. The formation of macroscopic jams will be described. The phase diagrams of the models on finite segments will be constructed. The statistics of avalanches in the interface growth "Raise and Peel model" will be studied. The probability of nonlocal configurations in the branching polymers or spanning trees models, their limit shapes and fluctuations in the scaling limit will be obtained. Statistics of the boundary of visited domain in the proposed in BLTP Eulerian walk model will be studied.

In addition to the studies of models of equilibrium and non-equilibrium statistical physics a major attention will be paid to the development of mathematical methods related to the theory of integrable systems, theory of phase transitions and conformal field theories. The theory of elliptic hypergeometric functions and integrals proposed in BLTP will be further developed. This theory gives the most modern mathematical apparatus for studies both the lattice and field theory models of physics of complex systems. The properties of elliptic Fourier transform necessary for an analysis of these models will be studied. The structure properties of quantum matrix algebras will be investigated, the differential geometry of quantum matrix groups will be developed. Concrete realizations and the representation theory of these objects, which are important building blocks of new integrable models of statistical and quantum physics, will be constructed.

List of activities: 2023

Results expected upon completion of the theme

Development of existing and creation of new theoretical methods and approaches for describing and predicting the properties of new materials, calculation of their characteristics and elucidation of the mechanisms that determine the behavior of such materials under their functionalization, structural changes, and the influence of external factors; identification of universal laws of behavior of equilibrium and nonequilibrium statistical systems; computer modeling of a wide class of twodimensional materials and revealing the possibility of creating various devices based on them; development of methods for studying strongly correlated systems; explanation of correlations between the structural characteristics of a wide class of materials and their physical properties.

Laboratory	N⁰N⁰	Name, Surname	N⁰N⁰	Name, Surname
BLTP	1	Anitas E.M.	18	Derbyshev A.E.
	2	Brankov J.	19	Pyatov P.N.
	3	Plakida N.M.	20	Kochetov E.A.
	4	Kuzemsky A.L.	21	Chizhov A.V.
	5	Yukalov V.I.	22	Shukrinov Yu.M
	6	Yushankhai V.Yu.	23	Katkov V.L.
	7	Cherny A.Yu.	24	Krasavin S.E.
	8	Slyamov A.M.	25	Maiti Moitry
	9	Tung Nguyen Dan	26	Plechko V.N.
	10	Vladimirov A.A.	27	Smotlacha J.
	11	Spiridonov V.P.	28	Rahmonov I.R.
	12	Inozemtsev V.I.	29	Kolesnikov D.V.
	13	Dubovik V.M.	30	Sadykova O.G.
	14	Zhidkov P.E	31 Kulikov K.V.	
	15	Ivanova T.A.	32	Medvedeva S. Yu.
	16	Papoyan V.V.	33	Glebov A.A.
	17	Bunzarova N.Zh.	34	Ivantsov I.D.
FLNP	1	Aksenov V.L.	3	Kozlenko D.P.
	2	Balagurov A.M.		
LIT	1	Zemlianaya E.V.	4	Syurakshina L.A.
	2	Sarhadov I.	5	Yukalova E.P.
	3	Serdyukova S.I.		
FLNR	1	Olejniczak A.		

Participants from JINR

Participating countries, institutes and organizations

Country or Organization	City	Institute or Laboratory	Participants Name, Surname	Status	
Azerbaijan	Baku	MSU (branch)	Nakhmedov E. +2	Exchange visits	
Armenia	Yerevan	YSU	Mardoyan L.G., Morozov V.F.	Collaboration	
		IIAP NAS RA	Pogosyan V.S.	Collaboration	
		Foundation ANSL	Izmailyan N.	Collaboration	
Belarus	Minsk	BSTU	Groda J. + 3	Exchange visits	
		IP NASB	Kilin S. +4	Exchange visits	

		SPC NASB	Saiko A. + 3	Exchange visits	
		ISEI BSU	Boyarkin O. + 4	Exchange visits	
		JIPNR-Sosny NASB	Kuvshinov V. + 2	Exchange visits	
Bulgaria	Sofia	IMech BAS	Bunzarova N.	Collaboration	
		INRNE BAS	Bananaeva B.	Collaboration	
		ISSP BAS	Tonchev N.	Collaboration	
			Chamati H. + 3		
		SU	Marvakov D.	Collaboration	
			Mishonov T.		
Vietnam	Hanoi	IMS VAST	Nguyen Van Hieu + 5	Exchange visits	
Mongolia	Ulaanbaatar	NUM	Lhagva O. + 2	Collaboration	
0		IPT	Sangaa D.	Exchange visits	
Poland	Warsaw	IPC PAS	Holas A., Olshevsky J.	Exchange visits	
	Wroclaw	TU	Mierzejewski M.	Collaboration	
	Katowice	US	Maska M.	Collaboration	
	Krakow	JU	Kaputzik E + 2	Exchange visits	
			Oles L.		
	Poznan	AMU	Navrocik W. + 1	Collaboration	
			Tanas M. + 3		
		IMP PAS	Morkowski J.	Exchange visits	
Russia	Moscow	ITEP	Khoroshkin S.M.	Exchange visits	
		MIRAS	Bogoliubov N.N. (jr)	Exchange visits	
		MIREA	Morozov V.G.	Collaboration	
		SINP MSU	Tolstoi V.N.	Exchange visits	
		NRNU "MEPhI"	Evseev I.V. + 3	Exchange visits	
		NRU HSE	Gritsenko V.A.	Exchange visits	
		NRCKI	Kagan Yu.M. + 3	Exchange visits	
		RUDN	Rybakov Yu.P. + 2	Collaboration	
	Troitsk	НРРІ	Tareeva E.E. + 2	Exchange visits	
	Belgorod	BSU	Chekanov N.A.	Collaboration	
	Voronezh	VSU	Zasorin Yu.V.	Collaboration	
	Gatchina	NRC KI PNPI	Ginzburg S.L.	Exchange visits	
			Maleev S.V. + 3		
	Kazan	KSU	Ignatiev Yu.G.	Collaboration	
	Protvino	IHEP	Saponov P.A., Razumov A.V.	Exchange visits	
	Samara	SGU	Saleev V.A., Shipilova A.V.	Collaboration	
	Saratov	SGU Glukhova O.E.+3		Collaboration	
			Kolesnikova A.S.		
	Perm	PSU	Henner V.K.	Collaboration	
	SPeterburg	PDMI RAS	Derkachev S.E.		
		SPBSTU	Antonov A.I.	Collaboration Collaboration	
		ETU	Sokolov A.I.	Collaboration	
			Antonov A.I.		
		II RAS	Shalaev B.N. + 1	Exchange visits	
Romania	Bucharest	IFIN-HH	Barsan V., Anghel D., Misicu	Protocol	
			S., Aranghel D.I		
	Cluj-Napoca	UTC-N	Szakacs Z., Todoran R.	Protocol	
	Timisoara	WUT	Bica I	Protocol	
			Papp E. + 1		
Slovakia	Bratislava	CU	Plecenic A.	Exchange visits	
	Kosice	PJ Safarik University	Ilkovic V.	Exchange visits	
		PJ Safarik University	Kalagov H.	Collaboration	
		IE PSAS	Pudlak M., Pincak R.	Exchange visits	
Uzbekistan	Tashkent	Assoc."PS." PTI	Abdullaev F. + 2	Exchange visits	
			Gulyamov K.		
Ukraine	Kiev	IMP NASU	Baryakhtar V.G. + 3	Exchange visits	
		NUK	Kadenko I.N.	Collaboration	

	L'viv	ICMP NASU	Стасюк И.В. + 3	Exchange visits	
	Kharkov	NSC KIPT	Peletminsky S.V. + 3	Exchange visits	
			Slezov V.V. + 2		
Czech Republic	Rez	NPI ASCR	Exner P., Dietrich J.	Exchange visits	
Hungary	Budapest	Wigner RCP	Zimani I. + 2	Exchange visits	
Germany	Braunschweig	TU	Scherm R.	Collaboration	
	Bonn	UniBonn	Rittenberg V.	Collaboration	
				Exchange visits	
	Bremen	UB	Chiholl G	Collaboration	
	Wuppertal	UW	Boos G., Geman F.	Collaboration	
			Klumper A.		
	Darmstadt	GSI	Nerenberg V. + 1.	Collaboration	
	Dortmund	TU Dortmund	Gerlach B. + 1	Collaboration	
	Dresden	IFW	Drechsler S. + 3	Agreement	
			Hozoi L.		
		MPI PkS	Fulde P., Meisner R.	Exchange visits	
		TU Dresden	Sahling S.	Agreement	
	Leipzig	UoC	Ben U., Ihle D.	Collaboration	
	Magdeburg	OVGU	Richter I.	Collaboration	
	Rostock	UR	Roepke G. + 2	Collaboration	
Italy	Catania	UniCT	Puchi R. + 2	Collaboration	
	Salerno	UNISA	Manchini F. + 3	Collaboration	
Australia	Melbourne	Univ.	de Geer J.	Collaboration	
	Sydney	Univ.	Molev A.	Collaboration	
Austria	Vienna	TU Wien	Brunner F.	Collaboration	
	Linz	JKU	Ernst A.	Collaboration	
Belgium	Louvain-la- Neuve	UCL	Ruele F. + 2	Collaboration	
Brazil	Brazilia	UnB	Oliveira F.	Exchange visits	
	Natal	IIP UFRN	Ferraz A.	Collaboration	
	Sao Paolo	USP	Bagnato V., Alcaraz F.	Exchange visits	
India	Mumbai	TIFR	Dhar D.	Collaboration	
Ireland	Dublin	DIAS	Dorlas T + 2	Exchange visits	
Spain	Madrid	ICMM-CSIC	Smirnov-Rueda R. + 1	Collaboration	
Canada	Quebec	UL	Kroeger H. + 3	Collaboration	
	Kingston	Queen's	Coleman A.	Collaboration	
	London	Western	Cottam M., Singh M.	Collaboration	
	Montreal	Concordia	Hall R.	Collaboration	
Serbia	Belgrade	INS "VINCA"	Galovic C., Cevizovic D.	Exchange visits	
Slovenia	Ljubljana	UL	Prelovsek P. + 3	Collaboration	
			Kabanov V.		
USA	Louisville	UofL	Henner V.	Exchange visits	
	New York	CUNY	Manassah J.	Exchange visits	
	Rochester	UR	Bigelow N.	Exchange visits	
	Tallahassee	FSU	Dzero M.	Collaboration	
Taiwan	Taipei	IP AS	Chin-Kun HU	Exchange visits	
France	Paris	UPMC	Zinn-Justin P.	Exchange visits	
	Annecy-le-	LAPTh	Chicherin D.	Collaboration	
	Vieux Valenciennes	UVHC	Gurevich D.	Exchange visits	
	Marseille	CPT	Ogievetskii O.	Collaboration	
	ividi seille	UPC	Zagrebnov V.	Agreement	
			Hein R.	Agreement	
	Nice	UN	Sornette D.	Exchange visits	
Switzerland	Villigen	PSI	Rosenfelder R.	Exchange visits	
	Zurich	ETH	Sornette D.	Collaboration	

Time frame of the theme: 2019-2023

Total estimated cost of the theme (thousand USD)

NN nn	Activities	Total cost	Costs per years 2019	2020	2021	2022	2023
1	Salary	4867,5	829,3	912,2	985,2	1044,3	1096,5
2	Social tax	1470,0	250,4	275,5	297,5	315,4	331,2
3	Social Security Fund	95,5	16,3	17,9	19,3	20,5	21,5
4	International cooperation	250,0	50,0	50,0	50,0	50,0	50,0
5	Materials	250,0	50,0	50,0	50,0	50,0	50,0
6	Equipment	400,0	80,0	80,0	80,0	80,0	80,0
	Total:	7333,1	1276,0	1385,6	1482,1	1560,2	1629,2
8	Infrastructure BLTP	2006,9	363,2	381,4	400,4	420,4	441,5
	TOTAL COSTS:	9340,0	1639,2	1767,0	1882,5	1980,6	2070,7
9	Infrastructure JINR	3361,6	608,4	638,8	670,7	704,3	739,5
	Total	12701,6	2247,6	2405,8	2553,2	2684,9	2810,1

Other financing sources

AGREED:

JINR Chief Scientific Secretary

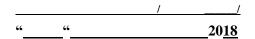
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Head of Planning and Finance Department

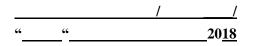
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Head of Science Organization Department

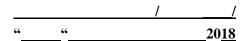
Laboratory Director



Laboratory Scientific Secretary



Laboratory Economist



Theme leaders