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 2019–2023

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. The results obtained will be used in carrying out experimental studies 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 two-dimensional materials on electronic transport are planned. In particular, effects such as electron-phonon 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 two-dimensional 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.

Participants from JINR

Laboratory	№№	Name, Surname	№№	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.	4	Kuklin A.I.
LIT	1	Zemlianaya E.V.	4	Syurakshina L.A.
	2	Sarhadov I.	5	Yukalova E.P.
	3	Serdyukova S.I.		
FLNR	1	Olejniczak A.		

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. Chamati H. + 3	Collaboration
		SU	Marvakov D. Mishonov T.	Collaboration
Vietnam	Hanoi	IMS VAST	Nguyen Van Hieu + 5	Exchange visits
Mongolia	Ulaanbaatar	NUM	Lhagva O. + 2	Collaboration
		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 Oles L.	Exchange visits
	Poznan	AMU	Navrocik W. + 1 Tanas M. + 3	Collaboration
		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	HPPI	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. Maleev S.V. + 3	Exchange visits
	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 Kolesnikova A.S.	Collaboration
	Perm	PSU	Henner V.K.	Collaboration
	S.-Peterburg	PDMI RAS	Derkachev S.E.	Collaboration
		SPBSTU	Antonov A.I.	Collaboration
		ETU	Sokolov A.I. Antonov A.I.	Collaboration
		II RAS	Shalaev B.N. + 1	Exchange visits
Romania	Bucharest	IFIN-HH	Barsan V., Anghel D., Misicu S., Aranghel D.I	Protocol
	Cluj-Napoca	UTC-N	Szakacs Z., Todoran R.	Protocol
	Timisoara	WUT	Bica I Papp E. + 1	Protocol
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."P.-S." PTI	Abdullaev F. + 2 Gulyamov K.	Exchange visits
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 Slezov V.V. + 2	Exchange visits
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. Klumper A.	Collaboration
	Darmstadt	GSI	Nerenberg V. + 1.	Collaboration
	Dortmund	TU Dortmund	Gerlach B. + 1	Collaboration
	Dresden	IFW	Drechsler S. + 3 Hozoi L.	Agreement
		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 Kabanov V.	Collaboration
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-Vieux	LAPTh	Chicherin D.	Collaboration
	Valenciennes	UVHC	Gurevich D.	Exchange visits
	Marseille	CPT	Ogievetskii O.	Collaboration
		UPC	Zagrebnov V. 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 пп	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

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Laboratory Director

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Laboratory Scientific Secretary

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Laboratory Economist

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"______"____________________2018

Theme leaders

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