Theme of BLTP "Theory of condensed matter" – REPORT

Theory of Condensed Matter
(2014-2018)

Leaders: **V.A. Osipov** and **A. M. Povolotsky**

Projects:

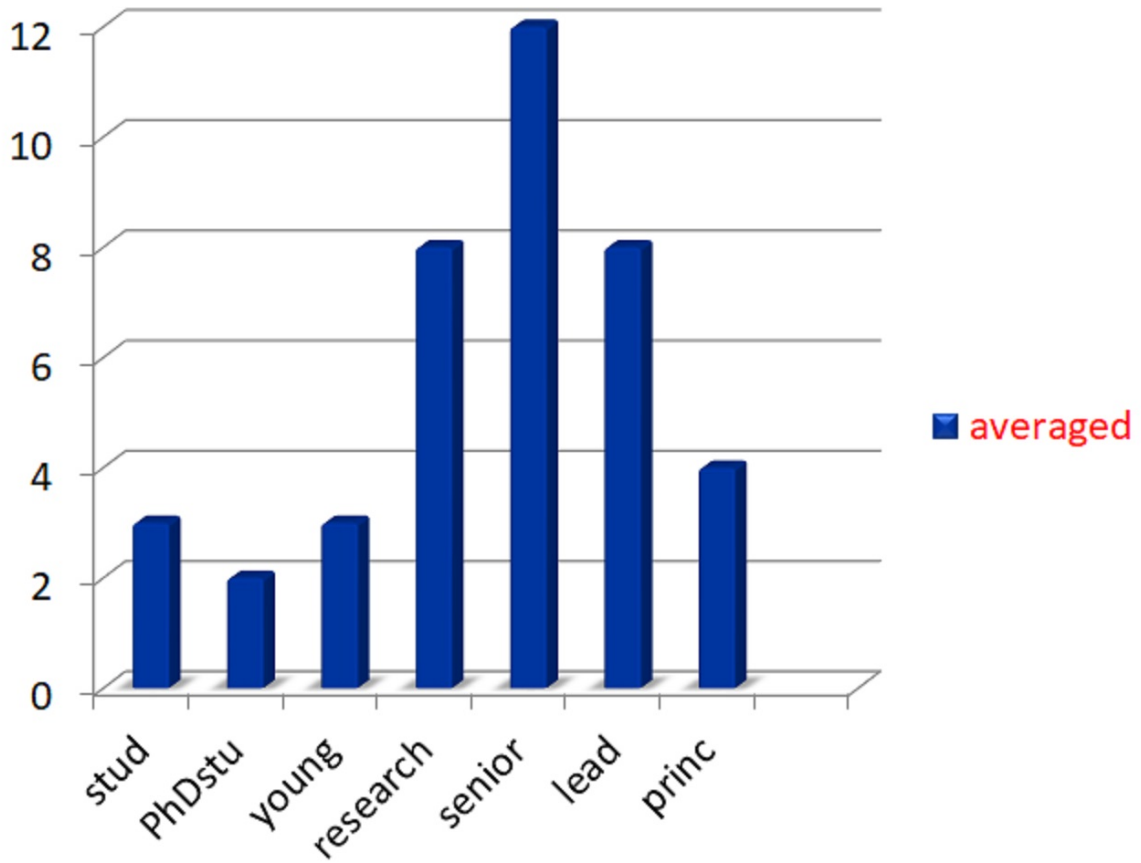
- Complex materials and nanostructures
- Spokespersons: **V.A. Osipov, N.M. Plakida**

- Contemporary problems of statistical physics
- Spokespersons: **A. M. Povolotsky, V.B. Priezzhev**

Theory of condensed matter – Main research topics

- Strongly correlated systems:
  high-temperature superconductors, colossal magneto-resistance compounds (manganites), heavy-fermion systems, low-dimensional quantum magnets with strong spin-orbit interaction, topological insulators (new hot topic)
- Physics of nanostructures:
  carbon nanostructures, quantum transport in molecular devices, spin dynamics of magnetic nanoclusters; fractal structures; layered superconductors and superconducting nanostructures in the external fields, resonance, radiative and chaotic properties of intrinsic Josephson junctions in high temperature superconductors
- Modern problems of statistical mechanics:
  exactly-solvable models of equilibrium and nonequilibrium statistical physics, phase transitions and critical phenomena, self-organized criticality, etc

Theory of condensed matter – PERSONNEL



- Doctors of science – **12**, Candidates of science (PhD) – **22**

Theory of condensed matter – International collaboration

International collaboration and long time positions at BLPT

- Russia – 25, Armenia – 2, Bulgaria – 2, Czechia – 2
- Kazakhstan – 1, Romania – 1, Slovakia – 1, Vietnam –1
- Tajikistan – 1, India – 1

Other participating countries

- Australia, Austria, Belgium, Brazil, Canada, Egypt, France, Germany, Hungary, India, Ireland, Italy, Serbia, Slovenia, South Africa, Spain, Switzerland, Taiwan, USA

Theory of condensed matter – Funding

- Direct financing from the budget of the Institute $--$ $2200k\$$ per year

- Subsidiary financing – Grants, projects and programs
  Azerbaijan Plenipotentiary at JINR
  Romanian Plenipotentiary at JINR
  Slovak Plenipotentiary at JINR
  Czech Plenipotentiary at JINR
  Ter-Antonyan - Smorodynsky program (Armenia-BLTP)
  Votruba-Blokhintsev program (Czech-BLTP)
  Heisenberg-Landau program (Germany-BLTP)
  RFBR, RNF (Russia)
  RFBR-DFG (Germany)
  RFBR-CNRS (France)

Theory of condensed matter – Scientific results

Publications (2014-until now)

- journals – 235
- books, chapters in books – 3
- review articles – 4
- conference proceedings – 37
- presentations at conferences – 64 (invited/oral) – 44 (posters)
- Nature Comm., PRL, PRB, APL, EPL, JETP Lett., JETP, J. Phys., JACR

Theory of condensed matter – Organization of Conferences, schools, workshops in BLTP

- International School Advanced Methods of Modern Theoretical Physics: Integrable and Stochastic Systems
  Č. Burdík (JINR & CTU), M. Hnatič (JINR)
- International conference Nucleation Theory and Applications
  J.W. P. Schmelzer and V.B. Priezzhev
- Forthcoming (July 9-12, 2018) international workshop Low-dimensional materials: theory, modeling, experiment
  V.A. Osipov

Theory of condensed matter – Organization of Conferences, schools, workshops in BLTP

Low-dimensional materials: theory, modeling, experiment

July 9-12
(Dubna, Russia)

About

The International workshop *"Low-dimensional materials: theory, modeling, experiment"* is organized by Bogoliubov Laboratory of Theoretical Physics, Joint Institute for Nuclear Research (JINR).

The workshop will cover the wide range of nanoscale phenomena in low-dimensional materials. The presentation will include oral talks and poster sessions.

Scientific program

2D materials: graphene and others
Nanoribbons and carbon nanotubes
Dirac and Weyl metals and semimetals
Transport phenomena in LDM
LDM-based heterostructures
LDM functionalization
LDM in nano/bio electronic devices

International Advisory Committee

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Organizing Committee

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V.L. Katkov - scientific secretary
O.M. Korotchik - secretary
A.A. Glebov
D.V. Kolesnikov
S.E. Krasavin
O.G. Sadykova

Location

The Workshop will be held in the *International Conference Center JINR Dubna*. Joint Institute for Nuclear Research is an international research organization involving more than 20 countries.

The institute activity embraces high-energy, nuclear and condensed matter physics. As an international recognition of JINR achievements, the element number 105 of the Periodic Table is called Dubnium in honor of the town Dubna.

Dubna is a small scientific town, 130 km north of Moscow, on the bank of the Volga river. There is a direct train and bus connection to Moscow.

The registration

The registration fee:

Participants	*120 EUR*
Students/accompanying persons	*80 EUR*

(Fee can also be paid in US dollars.)

Fee includes welcome party, coffee breaks, banquet, the publication book of abstracts, single fixed-time bus transfer between airport Sheremetyevo and Dubna on July 8 and 13. Some limited financial support might be possible on request preferably for young scientists from Russia and other JINR Member States and European countries.

For registration: http://indico.jinr.ru/event/bltp/ldm2018
E-mail: ldm2018@theor.jinr.ru

Number of participants is limited.
The end of registration and abstract deadline March 1, 2018

Theory of condensed matter – JINR Prizes

Theoretical physics research

- 2013 First Prize **Theory of Spin Fluctuations and High-Temperature Superconductivity in Cuprates**
  N. Plakida, S. Adam, G. Adam (LIT), **A. Vladimirov**, D. Ihle (Germany), V. Oudovenko (USA)
- 2014 First Prize **Superconformal Indices and Dualities in Four-Dimensional Supersymmetric Field Theory**
  V. Spiridonov, G. Vartanov
- 2017 First Prize **Strong electron correlations in underdoped high-temperature superconductors**
  A. Ferraz (Brazil), **I. Ivantsov, E. Kochetov**, M. Maśka, M. Mierzejewski (Poland)

Physics instruments and methods

- 2017 Second Prize **Structure of deterministic mass, surface and multiphase fractals: theory and methods of analysing the intensity of small-angle scattering**
  A. Cherny, E. Anitas, V. Osipov, A. Kuklin, M. Balasoiu (LNP)

Theory of condensed matter – JINR Prizes

- Patent: **Tunnel field-effect transistor on the base of graphene**
  V.L. Katkov, V.A. Osipov (Applied Physics Letters 104, 053102 (2014))

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РОССИЙСКАЯ ФЕДЕРАЦИЯ

ПАТЕНТ

НА ИЗОБРЕТЕНИЕ

№ 2554694

ТУННЕЛЬНЫЙ ПОЛЕВОЙ ТРАНЗИСТОР НА ОСНОВЕ ГРАФЕНА

Патентообладатель(ли): *Объединенный Институт Ядерных Исследований (RU)*

Автор(ы): *Катков Всеволод Леонидович (RU), Осипов Владимир Андреевич (RU)*

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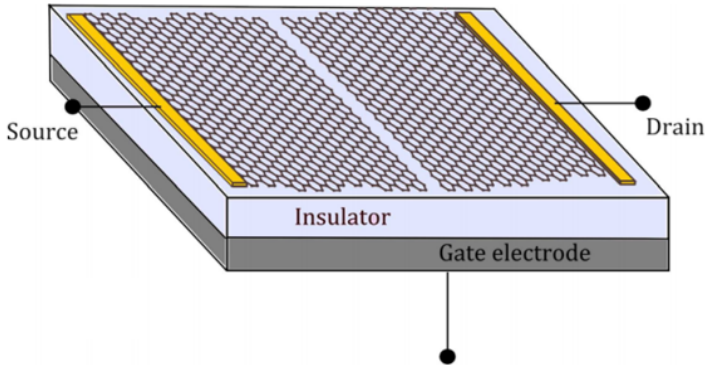
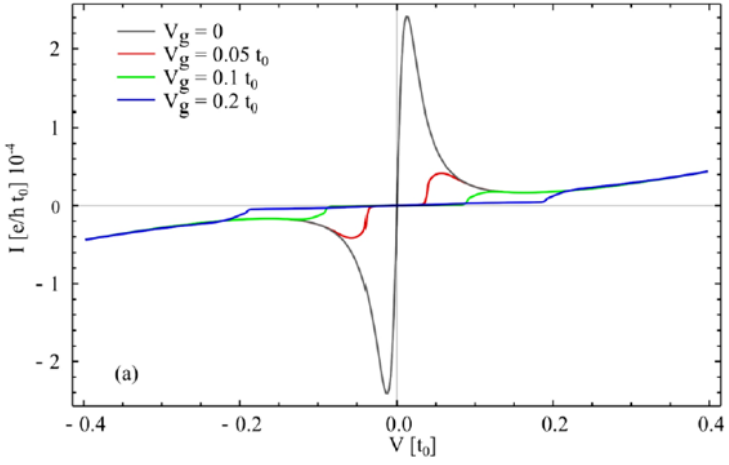
Врио руководителя Федеральной службы по интеллектуальной собственности
Л.Л. Кирий





Theory of condensed matter – Overview of research

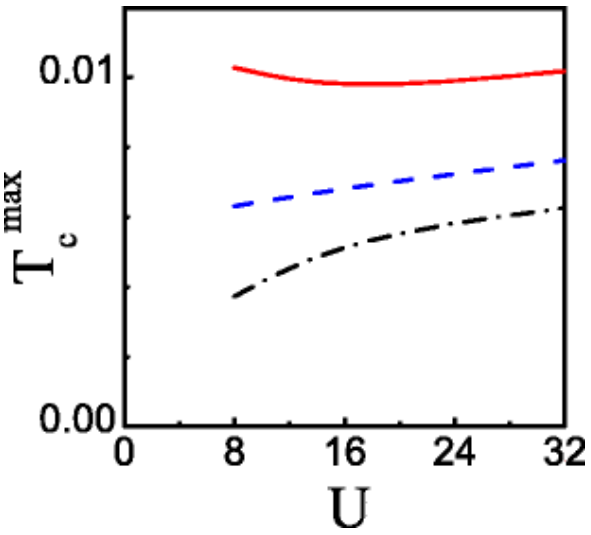
- **Orbital reconstruction in nonpolar tetravalent transition-metal oxide layers**
  N.A. Bogdanov, V.M. Katukuri, J. Romharnyi, **V. Yushankhai**, V. Kataev, B. Buechner, J. van den Brink & Liviu Hozoi
  NATURE Communications, v. 6, p. 7306 (2015)
- **Strongly frustrated triangular spin lattice emerging from triplet dimer formation in honeycomb Li2IrO3**
  S. Nishimoto, V. Katukuri, **V. Yushankhai**, H. Stoll, U. Roessler, L. Hozoi, I. Rousochatzakis, J. van den Brink
  NATURE Communications, v.7, p. 10273 (2016)

Consequences of a weak breaking of hexagonal structural symmetry in the lattice forming the sequence of magnetic layer is considered in layered iridium oxides. With the use of the computer codes for quantum-chemical cluster calculations in combination with methods of quantum many-particle theory, the authors developed original model of magnetic interactions. On this basis, they predicted theoretically the new type of magnetic ground state. The prediction can be verified by means of neutron diffraction and neutron magnetic spectroscopy.

Theory of High-Temperature Superconductivity in Cuprates

A microscopic theory of superconductivity for systems with strong electron correlations such as cuprates was proposed in the framework of the extended Hubbard model where the intersite Coulomb repulsion and electron-phonon interaction (EPI) are taken into account.

- **N.M. Plakida**, V.S. Oudovenko, Journal of Superconductivity and Novel Magnetism, **29**, 1037–1042

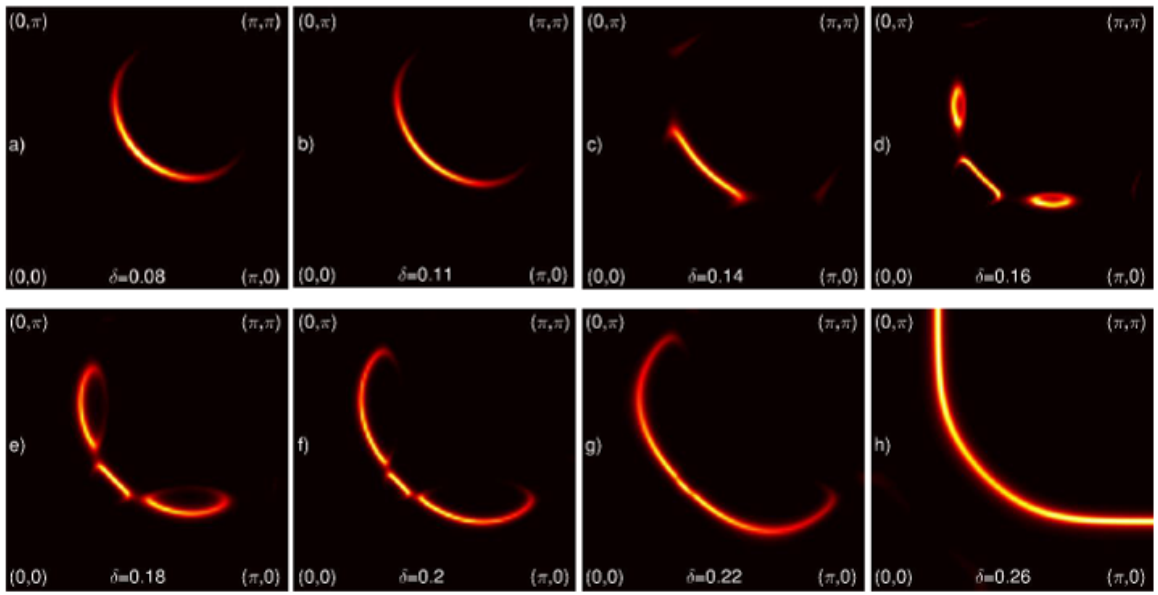


Maximum $T_c^{\max}$ at the optimal doping as a function of U for intersite Coulomb repulsion $V = 0.0$ (bold red line), $V = 0.5$ (blue dashed line), and $V = 1.0$ (black dash-dotted line)

Itinerand localized model of strongly correlated electrons: Fermi-surface reconstruction

- **I. Ivantsov,** A. Ferraz, **E. Kochetov**, Phys. Rev. B **96**, 195161 (2017)

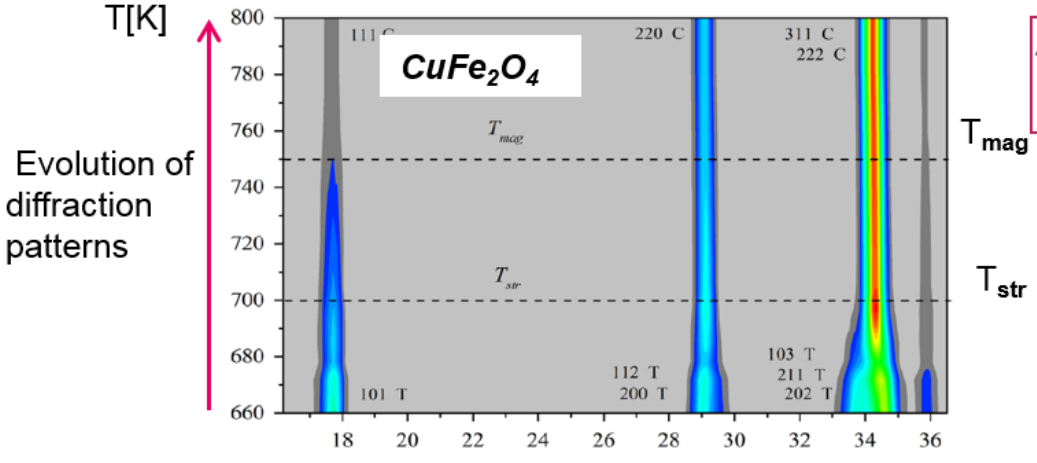
Unexpected behavior of the Fermi-surface of the high-temperature superconducting cuprates is explained in the framework of the t–J model on the base of strong electron correlations resulting in a charge density wave instability. For the first time, the results reproduce experimental data on the ordering in hole doped cuprates within the microscopic model.



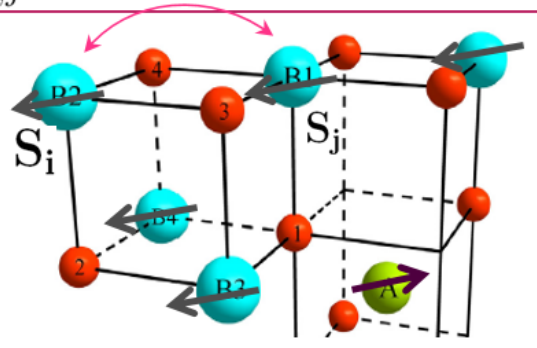
Observed Fermi-surface reconstruction: pseudogap phase (a–c); charge density wave (d–f); pseudogag (g); Fermi liguid (h).

Studies of magnetic and structure phase transitions with high resolution neutron diffraction and modern quantum models of magnetism

- A.M. Balagurov, I.A. Bobrikov, V. Yu. Pomjakushin, D.V. Sheptyakov, **V.Yu. Yushankhai**, JMMM **374**, 591 (2015)



$$\mathcal{H} = \sum_{i,j} J(\mathbf{r_i} - \mathbf{r_j})\mathbf{S_i}\mathbf{S_j} + \mathcal{H}_{Jahn-Teller}$$

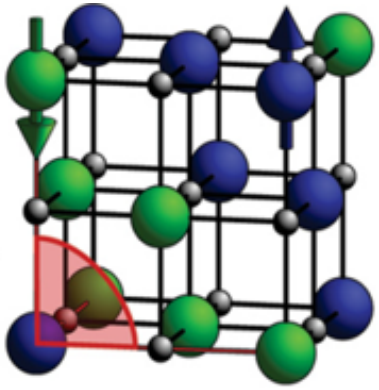


Studies of magnetic and structure phase transitions with high resolution neutron diffraction and modern quantum models of magnetism

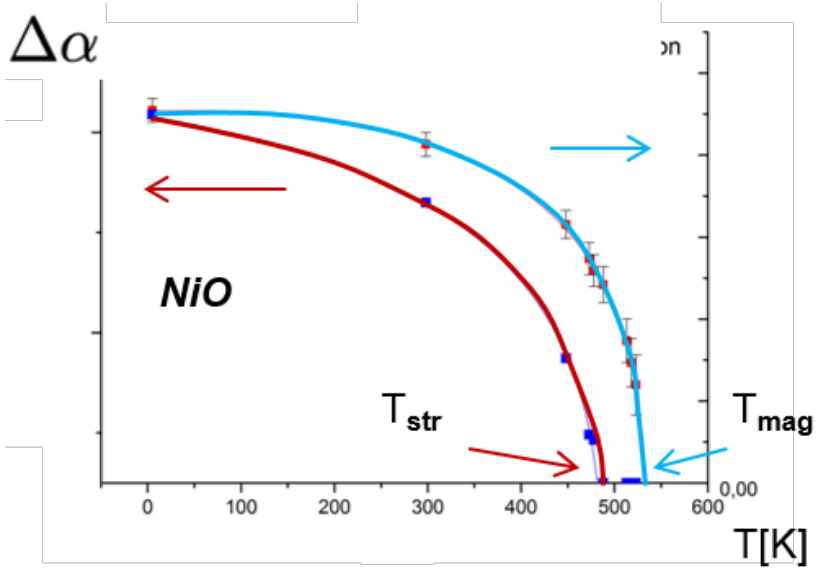
- A. Balagurov, I. Bobrikov, S. Sumnikov, **V. Yushankhai**, JETP Letters, **104**, 84 (2016)

$$T_{\mathrm{mag}} - T_{\mathrm{str}} = 50\ \mathrm{K}$$

NiO



$$\Delta\alpha = \alpha - 90^\circ$$

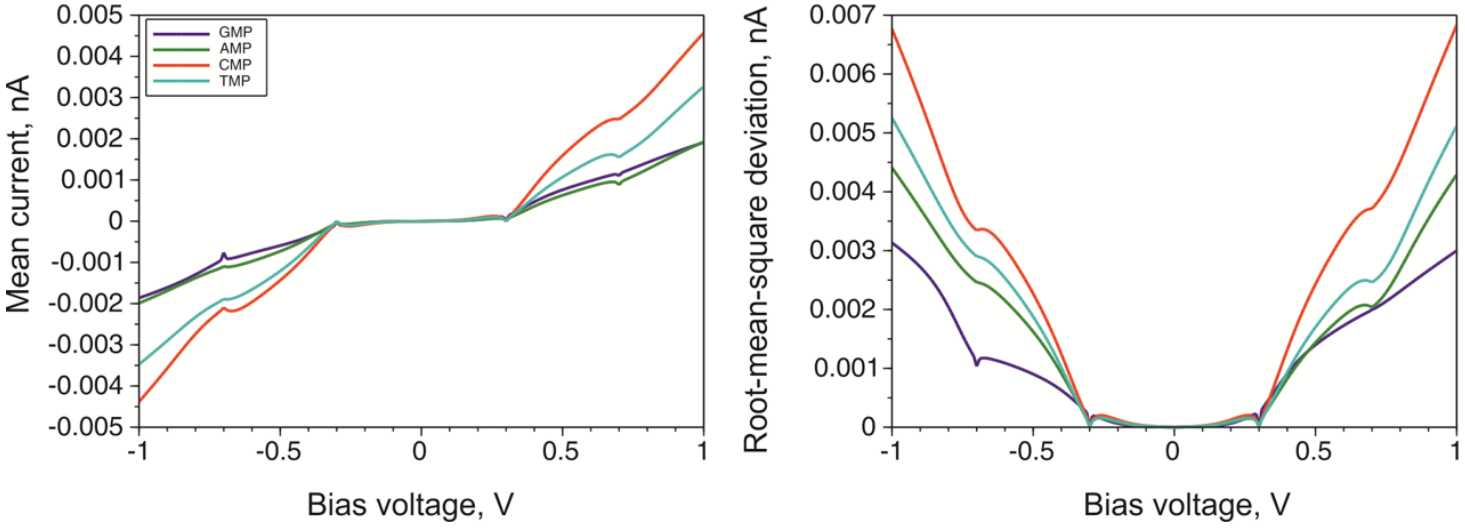


Separation of magnetic and structural ($\Delta\alpha \neq 0$) phase transitions observed in neutron experiments is explained in the framework of J_1–J_2 spin model and a generalization of the Landau theory for the case of weak interaction of two (magnetic and structural) order parameters.

A model of sequential electron transport in the system graphene-nucleotide-graphene. DNA decoding

- **O.G. Isaeva, V.L. Katkov, V.A. Osipov**, Eur. Phys. J. B **87**, 272 (2014)

An important role of measurement of specific for each nucleotide dispersion of current in addition to transverse current for DNA decoding is shown in the regime of sequential tunneling



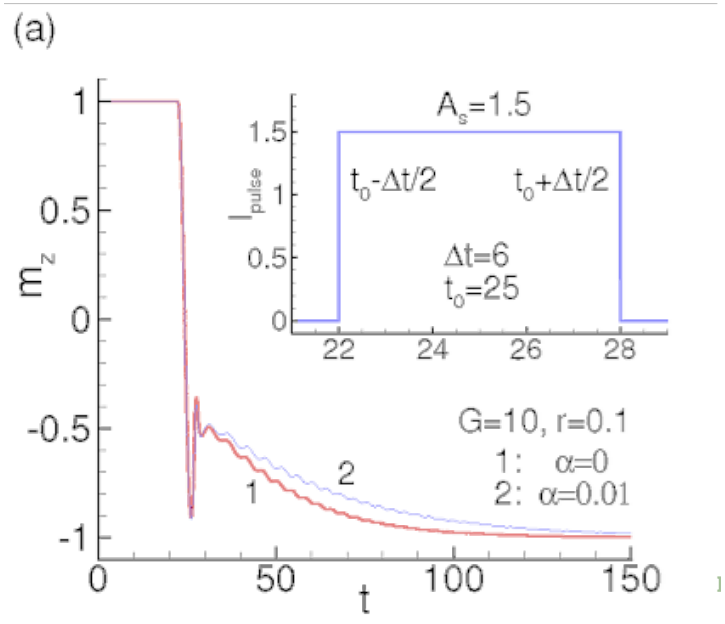
This result is illustrated with both I-V characteristics (left) averaged by different angular orientations and shifts of nucleotides in the nanogap plane and root mean square deviation vs voltage (right) obtained in the case of the same energetic parameters for each nucleotide.

Theory of condensed matter – Overview of research

Switching of magnetization under rectangular current pulse

- **Yu. M. Shukrinov**, **I. R. Rahmonov**,K. Sengupta, and A. Buzdin, Appl. Phys. Lett. **110**, 182407, (2017)

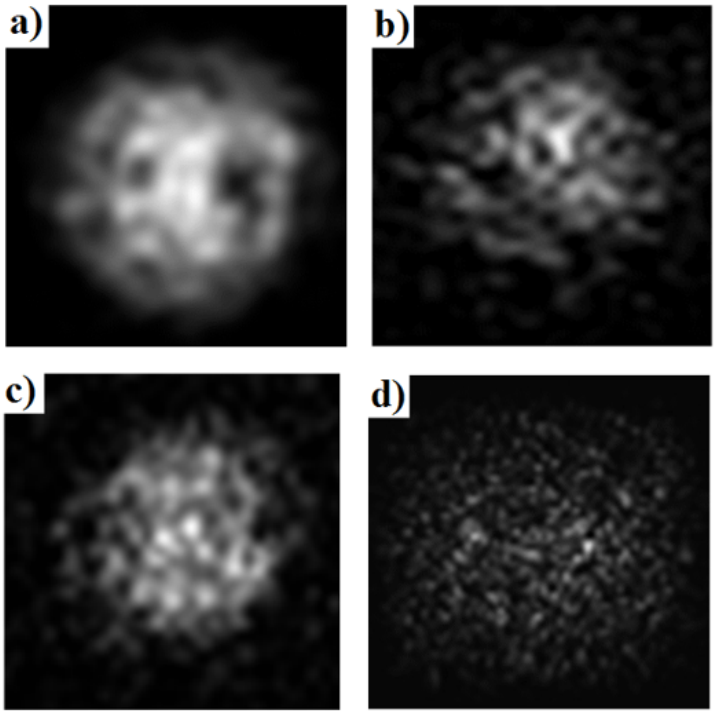
Magnetization reversal in a Josephson junction with direct coupling between magnetic moment and superconducting current is studied. Simulations of magnetic moment dynamics show that by applying an electric current pulse, we can realize the full magnetization reversal. Different protocols of full magnetization reversal based on the variation of the Josephson junction and pulse parameters have been proposed.



Theory of condensed matter – Overview of research

A new effect – Inverse Kibble-Zurek scenario – has been predicted and described theoretically, as well as confirmed by numerical simulations and experiments with cold trapped atoms

- **V.I. Yukalov**,A.N. Novikov, V.S. Bagnato, Laser Phys. Lett. **11**, 095501 (2014)
- A.N. Novikov, **V.I. Yukalov**, V.S. Bagnato, J. Phys. Conf. Ser. **594**, 012040 (2015)
- **V.I. Yukalov**,A.N. Novikov, and V.S. Bagnato, Phys. Lett. A **379**, 1366–1371 (2015)

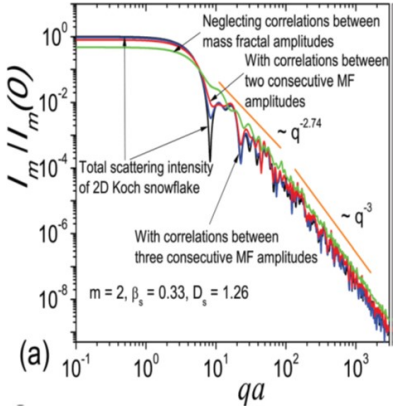


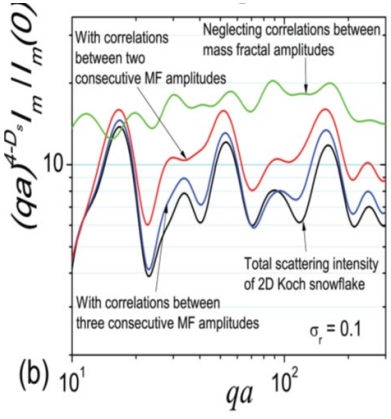
The sequence of nonequilibrium states realized in numerical modeling: (a) vortex state, (b) vortex turbulence, (c) grain turbulence, (d) wave turbulence. The density cross-sections are demonstrated. Brighter colour corresponds to higher density.

Small-angle scattering from deterministic surface fractals

- **A. Yu. Cherny**, **E. M. Anitas**, **V. A. Osipov**, A. I. Kuklin, J. Appl. Cryst. **50**, 919 (2017)
- **A. Yu. Cherny**, **E. M. Anitas**, **V. A. Osipov**, A. I. Kuklin, Phys. Chem. Chem. Phys. **19**, 2261 (2017)

New properties of fractals were predicted and a **new method for extracting structural information of fractals** from SAS – **the fractal iteration number**, **the scaling factor** was developed. Any **surface fractal is decomposed into mass-fractal iterations** of the same fractal dimension. It follows from this decomposition that the scattering amplitude of a surface fractal can be calculated as a sum of the mass fractal amplitudes. **SAS** from a **surface fractal** is explained in terms of a **power-law distribution of sizes** of objects composing the fractal.





(a) the total intensity (black) and the intensities taking into account various correlations between the mass fractal amplitudes; (b) Approximate log-periodicity of the scattering

Mathematical problems of many-particle systems

Emergence of jams in the generalized totally asymmetric simple exclusion process

- **A.E. Derbyshev**, **A.M. Povolotsky**, **V.B. Priezzhev**, Phys. Rev. E **91**, 022125 (2015)

A Loop Reversibility and Subdiffusion of the Rotor-Router Walk

- **Vl.V. Papoyan**, **V.S. Poghosyan**, **V.B. Priezzhev**, Journal of Physics A: Mathematical and Theoretical (2015)

A model of jam formation in congested traffic

- **N.Zh. Bunzarova**, **N.C. Pesheva**, **V.B. Priezzhev**, **J.G. Brankov**, Physica A: Statistical Mechanics and its Applications **494**, 340–350 (2018)

New elliptic solutions of the Yang–Baxter equation

- D. Chicherin, S.E. Derkachov, **V.P. Spiridonov**, Communications in Mathematical Physics **345** (2), 507–543 (2016)

Theory of condensed matter – Reports at PAC meetings

- Graphene-based tunnel junction V. Katkov (2015)
- The poster selected as the best poster at the session A model of sequential electron transport in the graphene-nucleotide-graphene system. DNA decoding O. Isaeva (2015)
- Proposal by BLTP for the JINR 7-Year Development Plan (2017–2023) in the field of condensed matter physics research M. Hnatic (2015)
- Quantum models of magnetism in strongly correlated electron systems with strong spin-orbit interaction V. Yushankhai (2015)

Theory of condensed matter – Reports at PAC meetings

- Discussion of the Draft Seven-Year Plan for the Development of JINR (2017–2023) in the field of condensed matter physics: Proposals by BLTP A. Povolotsky (2016)
- Novel features of Josephson nanostructures under external electromagnetic radiation (Results of collaboration with Germany, Slovakia, South Africa, Egypt, Japan, India, and Tajikistan) Yu. Shukrinov (2016)
- Fermi surface reconstruction in underdoped cuprates E. Kochetov (2017)
- Planar graphene tunnel field-effect transistor: effect of edge vacancies on performance V. Katkov (2018)

Theory of condensed matter – New theme – Motivation

Research in the last years was done in several main directions:

- Purely fundamental research based on long-term experience of BLTP in fields of solid state physics and statistical systems
- There is a commitment to work on problems directly related to contemporary experimental research, and consequently there is a direct communication between our theoreticians not only with experimental physicists from JINR laboratories, but experimental physicists from member states
- Moreover, there is a desire to use our long-term experience and methodics developed by our theoreticians in research of new materials, for example graphenes etc., with possibility to model real devices.

Theory of condensed matter – New theme – Motivation

All of these new tendencies are considered in formulation of new theme objectives, which are formulated on the base of the following principles:

- To preserve and further advance the traditional fundamental research in fields of solid state physics and statistical mechanics
- Simultaneously to not neglect the possibility to pursue the theoretical research of more pragmatic themes linked to research of new materials, such as for example nanostructures and nanomaterials
- And of course to contribute to hot topics – to still not properly researched and understood fundamental phenomena, such as for example high-temperature superconductivity
- These new tendencies and commitments are also reflected in naming of the new theme, which should sufficiently enough reflect the essence of our research in the next 5 years and follow up continuously on the old theme.

Theory of Complex Systems and Advanced Materials

Leaders: V.A. Osipov, A.M. Povolotsky

Projects:

- Complex materials
  Spokespersons: E. Anitas, N.M. Plakida
- Nanostructures and nanomaterials
  Spokespersons: V.A. Osipov, E.A. Kochetov
- Mathematical models of statistical physics of complex systems
  Spokespersons: A.M. Povolotsky, J. Brankov

Complex materials

- A combined theoretical and experimental (LNP) study of effects of high pressure on the structural, electronic and magnetic properties of heavy rare-earth metals
- Theoretical and experimental (LNP) investigations of the structure of complex hierarchical systems, including surface fractals and multifractals
- 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
- 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.
- 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.

Nanostructures and nanomaterials

- Theoretical investigations of electronic and transport properties of two-dimensional materials: graphene, phosphorene, silicene, and others
- 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
- Theoretical analysis of the physical properties of fluorinated and oxidized graphene (experiments in FLNR)
- Investigations of resonance, chaotic and topological features of Josephson nanostructures and superconducting devices

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, close collaboration with LIT JINR is planned, primarily by using the supercomputer "Govorun".

Mathematical models of statistical physics of complex systems

- Studies of statistics of particle flows on the lattices in stochastic models like exclusion processes with generalized interactions, zero-range processes and avalanche processes. 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.

Theory of Complex Systems and Advanced Materials – Funding

- Budget: Total expenses for 5 years: 12 700 000 USD
- structure of budget - salary, international cooperation, materials, equipment, infrastructure BLTP
- Subsidiary financing: Grants, Projects, Programmes – USD

Thank you for your attention