STAT PHYS 2019

5-th Conference on Statistical Physics: Modern Trends & Applications

Dedicated to the 110th anniversary of the birth of M.M.Bogolyubov

Book of abstracts

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July 3-6, 2019
Lviv, Ukraine

The 5th Conference

Statistical Physics: Modern Trends and Applications

3–6 July 2019, Lviv, Ukraine

Dedicated to the 110th anniversary of the birth of M.M. Bogolyubov

PROGRAMME AND ABSTRACTS

Lviv – 2019

The 5-th Conference "Statistical Physics: Modern Trends and Applications" will be held on July 3–6, 2019, in Lviv, Ukraine. This Conference continues a tradition of regular international meetings in the statistical physics in Ukraine, established in the 1970-ies and renewed by "Statistical Physics" (Lviv, 2005; Kharkiv, 2006; Lviv, 2009 and Lviv, 2012).

The 5-th Conference "Statistical Physics: Modern Trends and Applications" is organized by the Institute for Condensed Matter Physics of the National Academy of Sciences of Ukraine (Lviv, Ukraine) and is dedicated to the 110-th anniversary of Academician M.M. Bogolyubov (1909–1992) and to the 50-th anniversary of the Lviv Department for Statistical Theory of Condensed States of the Bogolyubov Institute for Theoretical Physics, which gave origin to the Institute for Condensed Matter Physics.

The Conference will consist of invited lectures (40 min.), keynote and contributed talks (15–25 min.) and poster presentations. Official language of the Conference is English.

A two-day tour to the Carpathian Mountains (the Transcarpathian region) will take place after the end of the conference on July 7–8 (Sunday–Monday).

Main topics

- Soft Matter Theory
- Quantum Statistics
- Computer Simulations
- Complex Systems

Contacts

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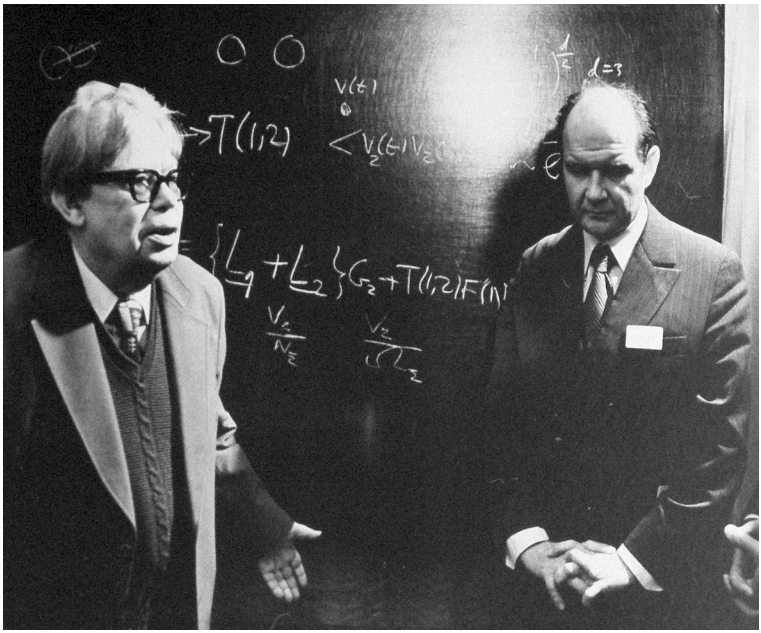

M.M. Bogolyubov and I.R. Yukhnovskii.

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of the National Academy of Sciences of Ukraine
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Conference History

This Conference continues a tradition of the regular workshops in the statistical physics in Ukraine, established in the 1970-ies and renewed by:

- **"Statistical Physics 2005: Modern Problems and New Applications"**, August 28–30, 2005, Lviv, Ukraine.
- **"Statistical Physics 2006. Condensed Matter: Theory and Applications"**, September 11–15, 2006, Kharkiv, Ukraine (dedicated to the 90th birthday of Ilya Lifshitz, founder of Condensed Matter Theory in Kharkiv).
- **The 3rd Conference "Statistical Physics: Modern Trends and Applications"**, June 23–25, 2009, Lviv, Ukraine (dedicated to the 100th birthday of the famous theoretical physicist and mathematician Mykola Bogolyubov and to the 40th anniversary of the Department of Statistical Theory of Condensed States of Institute for Theoretical Physics (Kyiv), which formed the basis of the Institute for Condensed Matter Physics).
- **The 4th Conference "Statistical Physics: Modern Trends and Applications"**, July 3–6, 2012, Lviv, Ukraine (dedicated to the 140th anniversary of the birth of Marian Smoluchowski, whose scientific activity was closely related to Lviv University, where he worked since 1899 and held the chair of theoretical physics in 1903–1913).

III CONIN Workshop:
Systems with competing electrostatic and short-range interactions

1–2 July 2019, Lviv, Ukraine

The workshop is organized as a part of the Horizon 2020 Marie Skłodowska-Curie Research and Innovation Staff Exchange project "Effects of confinement on inhomogeneous systems" (CONIN). In the CONIN project, modelling of self-assembly in systems with competing interactions as well as modelling of systems with dominant electrostatic interactions is planned. The project involves seven research institutions in Europe and South America:

- Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw, Poland (Coordinator);
- Institute of Physical Chemistry ROCASOLANO, CSIC, Madrid, Spain;
- Chimie ParisTech, Paris, France;
- Institute for Condensed Matter Physics, National Academy of Sciences of Ukraine, Lviv, Ukraine;
- Sorbonne University, Paris, France;
- University of La Plata, Argentina;
- Belarusian State Technological University, Minsk, Belarus.

The aim of the III CONIN workshop is to summarize the recent progress in colloidal and amphiphilic self-assembly and in the room temperature ionic liquids, both in the bulk and in confinement, as well as in mobile ions in intercalation compounds and on solid surfaces. Recent advances in theoretical and simulation methods appropriate for inhomogeneous systems, and in experimental studies of such systems will be presented. Review lectures by invited outstanding theoreticians and experimentalists and by senior researchers participating in the project are planned. In addition, there will be a poster session.

The previous workshops were held in Jablonna Palace in Warsaw in February 2017 and in Madrid in March 2018.

The 5th Conference

"Statistical Physics: Modern Trends and Applications"

Programme

3–6 July 2019, Lviv, Ukraine

Wednesday, July 3, 2019

Lviv Polytechnic National University, main building, Mateyko hall

9:00 – 13:00 Registration of the "StatPhys-2019" participants

13:00 – 13:10 OPENING CEREMONY

Chaired by I. Mryglod *(Lviv, Ukraine)*

13:10 – 13:35 A. Trokhymchuk *(Lviv, Ukraine)*
Leopolis Scientifica: Scientific heritage versus modern trends in statistical physics

13:35 – 14:15 A. Ciach *(Warsaw, Poland)*
Density functional theory for systems with competing interactions

14:15 – 14:40 O. Bakai *(Kharkiv, Ukraine)*
Three-state mesoscopic model of a heterophase fluid in application to the dielectric-semiconductor transformations in expanded mercury

14:40 – 14:55 O. Pizio *(Mexico City, Mexico)*
On the phase behavior of water-like fluids with square-well attractions and site-site association in slit-like pores. Density functional approach

14:55 – 15:10 J. Paturej *(Dresden, Germany)*
Universal equation of state for polymer solutions

15:10 – 15:40 Coffee Break

Chaired by O. Derzhko *(Lviv, Ukraine)*

15:40 – 16:20 J. Freericks *(Washington, USA)*
A primer on quantum computing for condensed matter physicists

16:20 – 17:00 I. Rousochatzakis *(Loughborough, United Kingdom)*
Quantum spin liquid at finite temperatures

17:00 – 17:25 J. Strečka *(Košice, Slovakia)*
Bound magnon crystals of spin-1/2 Heisenberg diamond and octahedral chains as a statistical-mechanical monomer-dimer problem

17:25 – 17:40 T. Domanski *(Lublin, Poland)*
From Bogoliubov to Majorana quasiparticles in topological superconductors

17:40 – 17:55 V. Tkachuk *(Lviv, Ukraine)*
Zeros of partition function and observables

17:55 – 18:15 Conference photo

18:30 – 21:00 GET-TOGETHER PARTY

Thursday, July 4, 2019

Lviv Polytechnic National University, main building, Mateyko hall

Chaired by C. Pierleoni *(L'Aquila, Italy)*

9:00 – 9:40 G. Ciccotti *(Rome, Italy)*
Dynamical Non-Equilibrium Molecular Dynamics

9:40 – 10:05 S. Bonella *(Lausanne, Switzerland)*
Approximate statistical properties of quantum nuclei via Generalised Langevin Dynamics

10:05 – 10:30 R. Davidchack *(Leicester, United Kingdom)*
Surface free energy of a hard-sphere fluid at curved walls: deviations from Morphometric Thermodynamics

10:30 – 10:45 H. Xu *(Metz, France)*
Stress fluctuations, shear modulus and phase transitions

10:45 – 11:00 A. Vidybida *(Kyiv, Ukraine)*
Stochastic mechanism for improving selectivity of olfactory projection neurons

11:00 – 11:30 Coffee break

Chaired by J. Kozicki *(Lublin, Poland)*

11:30 – 12:10 R. Kenna *(Coventry, United Kingdom)*
From the Ising model to sociophysics and back again — via the humanities: My adventures in a distant academic world

12:10 – 12:50 J. Sznajd *(Wroclaw, Poland)*
Magnetic phase transition induced by an electric field

12:50 – 13:15 M.A.F. Sanjuán *(Madrid, Spain)*
Basin entropy and testing for Wada basins to analyze the unpredictability of some physical systems

13:15 – 13:30 M. Dudka *(Lviv, Ukraine)*
Self-averaging in the two-dimensional random-bond Ising model

13:30 – 15:00 Lunch

Chaired by A. Ciach *(Warsaw, Poland)*

15:00 – 15:40 G. Kahl *(Wien, Austria)*
The physics of dendrimer-like DNAs: simulation and experiment

15:40 – 16:05 W. Góźdź *(Warsaw, Poland)*
Systems with competing interactions under confinement

16:05 – 16:20 V. Vikhrenko *(Minsk, Belarus)*
Influence of interparticle correlations on electrophysical properties of solid electrolytes

16:20 – 16:50 Coffee break

Chaired by N. Ivanov *(Sophia, Bulgaria)*

16:50 – 17:30 J. Richter *(Magdeburg, Germany)*
The challenge of highly frustrated quantum magnets at finite temperatures

17:30 – 17:55 J. Schnack *(Bielefeld, Germany)*
High spin cycles: Topping the spin record for a single molecule verging on quantum criticality

18.00 – 19.30 POSTER SESSION

Chaired by: A. Belonoshko *(Stockholm, Sweden)*
J. Freericks *(Washington, USA)*
G. Kahl *(Wien, Austria)*
M. Dudka *(Lviv, Ukraine)*

Friday, July 5, 2019

Lviv Polytechnic National University, main building, Mateyko hall

Chaired by J. Richter *(Magdeburg, Germany)*

9:00 – 9:40 S. Flach *(Daejeon, South Korea)*
Dynamical glass

9:40 – 10:05 M. Haque *(Maynooth, Ireland)*
Eigenstate thermalization for local and nonlocal operators

10:05 – 10:30 O. Kolezhuk *(Kyiv, Ukraine)*
Fidelity at Berezinskii–Kosterlitz–Thouless transitions

10:30 – 10:45 V. Pastukhov *(Lviv, Ukraine)*
Finite-momentum impurity in one-dimensional Bose gas

10:45 – 11:00 A. Sotnikov *(Kharkiv, Ukraine)*
Ferromagnetism of $LaCoO_3$

11:00 – 11:30 Coffee break

Chaired by G. Ciccotti *(Rome, Italy)*

11:30 – 12:10 A. Seitsonen *(Paris, France)*
Computer simulations of liquids and solvation using density functional theory-based molecular dynamics: Liquid water

12:10 – 12:35 O. Kalugin *(Kharkiv, Ukraine)*
Mixtures of room temperature ionic liquids with molecular solvents: challenge for the molecular modelling techniques

12:35 – 13:00 N. Jakse *(Grenoble, France)*
Dynamic heterogeneities in undercooled metallic alloys: An ab initio molecular dynamics study

13:00 – 13:15 J.-F. Wax *(Metz, France)*
Ab-initio molecular dynamics study of the pressure dependence of the collective excitations in liquid Ga-Sb alloy

13:15 – 13:30 M. Lukšič *(Ljubljana, Slovenia)*
Interpolation scheme for accurate predictions of PMFs and dielectric constants of electrolyte solutions. The use in implicit solvent simulations

13:30 – 15:00 Lunch

Chaired by G. Ruocco *(Rome, Italy)*

15:00 – 15:40 C.Pierleoni *(L'Aquila, Italy)*
Liquid-liquid transition in high pressure hydrogen by Quantum Monte Carlo methods

15:40 – 16:05 A. Belonoshko *(Stockholm, Sweden)*
Viscosity of the Inner Core

16:05 – 16:20 O. Rebenko *(Kyiv, Ukraine)*
Correlation of clusters: partially truncated correlation functions and their decay

16:20 – 16:50 Coffee break

Chaired by S. Flach *(Daejeon, South Korea)*

16:50 – 17:15 A. Honecker *(Cergy-Pontoise, France)*
Thermodynamics of the 2D $S = 1/2$ Shastry–Sutherland model and $SrCu_2(BO_3)_2$

17:15 – 17:30 V. Cheranovskii *(Kharkiv, Ukraine)*
Quantum phase transitions and intermediate magnetization plateau of 1D Heisenberg spin systems

17:30 – 17:45 O. Hryniv *(Durham, United Kingdom)*
Statistics of phase boundaries: renormalisation and sharp asymptotics

17:45 – 18:00 V. Gerasimenko *(Kyiv, Ukraine)*
Processes of creation and propagation of correlations in quantum many-particle systems

18:00 – 19:45 EXCURSION

20:00 – 23:00 CONFERENCE DINNER

Saturday, July 6, 2019

Lviv Polytechnic National University, main building, Mateyko hall

Chaired by N. Jakse *(Grenoble, France)*

9:00 – 9:40 G. Ruocco *(Rome, Italy)*
Probing the non-Debye low-frequency excitations in glasses through fast quenching and random pinning

9:40 – 9:55 A. Krivchikov *(Kharkiv, Ukraine)*
Thermal conductivity universality of disorder solids and complex crystals

9:55 – 10:25 L. Ponomarenko *(Lancaster, United Kingdom)*
Two-dimensional superlattices: from atomic planes to practical devices

10:25 – 10:45 J. Kozicki *(Lublin, Poland)*
Quantum stabilization and phase transitions in quantum anharmonic crystals

10:45 – 11:00 V. Ohanyan *(Yerevan, Armenia)*
Non-conserved magnetization, negative *g*-factors and 'fire-and-ice' spin configurations

11:00 – 11:30 Coffee break

Chaired by Yu. Kalyuzhnyi *(Lviv, Ukraine)*

11:30 – 12:10 M. Saphiannikova *(Dresden, Germany)*
Modeling of field-controllable polymers for mechanical applications

12:10 – 12:50 D. di Caprio *(Paris, France)*
Simple lattice model approaches in electrochemistry

12:50 – 13:15 S. Sokołowski *(Lublin, Poland)*
Density functional theory for nanoparticles at liquid-liquid interfaces

13:15 – 13:30 S. Kondrat *(Warsaw, Poland)*
Fluid-mediated interactions between colloids in bulk and under confinement

13:30 – 15:00 Lunch

Chaired by R. Kenna *(Coventry, United Kingdom)*

15:00 – 15:40 A. Dutech *(Nancy, France)*
Deep Reinforcement Learning: sometimes it works, more often it doesn't!

15:40 – 16:05 M. Koch-Janusz *(Zurich, Switzerland)*
Information theory, machine learning and the renormalization group

16:05 – 16:20 M. Druchok *(Lviv, Ukraine)*
Material design assisted by machine learning

16:20 – 16:45 K. Kułakowski *(Cracow, Poland)*
Towards the Heider balance — asymmetric social relations

16:45 – 17:00 CLOSING CEREMONY

LIST OF POSTERS

1. V. Baliha *(Lviv, Ukraine)*
   Quantum Heisenberg antiferromagnet on frustrated bilayer lattices

2. S.D. Balika *(Odesa, Ukraine)*
   Electrical conductivity of suspensions of particles with thin electric double layers

3. O. Baran *(Lviv, Ukraine)*
   One-dimensional XY model of magnetoelectric in the presence of an energy current

4. V. Blavatska *(Lviv, Ukraine)*
   On the shape of invading population in oriented environments

5. M.S. Bulakhov *(Kharkiv, Ukraine)*
   Role of nonlocal interaction in theory of a weakly non-ideal Bose gas with condensate

6. R.L. Davidchack *(Leicester, UK)*
   Direct calculation of surface free energy of mannitol by Molecular Dynamics simulations

7. T. Demchuk *(Lviv, Ukraine)*
   Shear stress correlations and collective excitations in liquid In via ab initio computer simulations

8. O. Derzhko *(Lviv, Ukraine)*
   Lattice-gas model of two-component fluid

9. O.A. Dobush *(Lviv, Ukraine)*
   Phase behavior of a cell fluid model with a modified Morse potential

10. O.A. Dobush *(Lviv, Ukraine)*
    Critical behavior of a supercritical cell fluid

11. D. Dobushovskyi *(Lviv, Ukraine)*
    Influence of the correlated hopping on the X-ray photoemission spectr

12. T.C. Dorlas *(Dublin, Ireland)*
On Dobrushin's uniquess theorem

13. Yu. Dublenych *(Lviv, Ukraine)*
Ground states of a system of classical spins on an anisotropic triangular lattice and the spin-liquid problem in $NiGa_2S_4$ and $FeGa_2S_4$ compounds

14. D.S. Dudariev *(Kharkiv, Ukraine)*
An influence of an effective cation charge on the microscopic structure and solvation dynamics in non-aqueous media

15. E. Ezerskaya *(Kharkiv, Ukraine)*
Low temperature thermodynamics of one-dimensional exactly solvable spin models with impurities

16. Ya.I. Filatov *(Kharkiv, Ukraine)*
Self-diffusion in the $BmimPF_6$/TfO-AN mixtures as seen by the quasi-elastic neutron scattering technique

17. O. Gaiduchok *(Lviv, Ukraine)*
Models of economical process based on econophysics laws

18. A. Glushchenko *(Kharkiv, Ukraine)*
Classification of the equilibrium state of magnetic media with spin $s = 3/2$ and SU(4) symmetry of exchange interaction

19. Kh.P. Gnatenko *(Lviv, Ukraine)*
Time-dependent correlation functions of q-deformed Bose gas and Fisher zeros

20. V. Gorev *(Dnipro, Ukraine)*
On the temperature evolution of a dissipative randomly driven system

21. K. Haydukivska *(Lviv, Ukraine)*
Universal features of complex n-block copolymers

22. P. Hlushak *(Lviv, Ukraine)*
Unification of thermo field kinetic and hydrodynamics approaches in the theory of dense quantum field systems

23. Yu. Honchar *(Kyiv, Ukraine)*
Resummation of ε-expansion for co-polymer star exponents reveals the order of the phase transition in thermal denaturation of DNA

24. T. Hutak *(Lviv, Ukraine)*
Thermodynamics of the $S = 1$ Heisenberg antiferromagnet on kagome lattice

25. T. Hutak *(Lviv, Ukraine)*
Low-temperature peculiarities of thermodynamic quantities for decorated spin chains

26. M. Hvozd *(Lviv, Ukraine)*
Fluid-fluid phase behaviour in the explicit hard spherocylinder solvent ionic model confined in a disordered porous medium

27. T. Hvozd *(Lviv, Ukraine)*
Two- and three-phase equilibria of polydisperse colloidal mixtures in bulk and random porous media

28. V. Ignatyuk *(Lviv, Ukraine)*
Nonequilibrium correlations in open quantum dynamics

29. J. Ilnytskyi *(Lviv, Ukraine)*
Aggregation and self-assembly of decorated nanoparticles by coarse-grained molecular dynamics simulations

30. N.B. Ivanov *(Sofia, Bulgaria)*
Frustrated Heisenberg spin models defined on a kagome-lattice strip

31. O. Kalyuzhnyi *(Lviv, Ukraine)*
Universal shape properties of mesoscopic polymer chains, polymer stars and their aggregates

32. K. Karľová *(Košice, Slovakia)*
Stepwise magnetization curves and bipartite entanglement of an exactly solvable spin-1/2 Ising–Heisenberg branched chain

33. A. Kats *(Odessa, Ukraine)*
Global isomorphism between Buckingham and Yukawa fluids and lattice gas

34. A. Khomenko *(Sumy, Ukraine)*
Modeling of noise effect on self-similar mode of ice surface softening during friction

35. O.V. Kliushnychenko *(Kyiv, Ukraine)*
Collective scattering of gas stream by impurity clusters: wake-mediated interaction, post-soliton structures and disorder-enhanced shock waves

36. Ya. Korduba *(Lviv, Ukraine)*
Public transportation networks as complex systems: between data processing and statistical physics

37. M. Korvatska *(Lviv, Ukraine)*
Diffusion of hard sphere fluids in a disordered porous media from generalized Enskog theory

38. N.A. Korynevskii *(Lviv, Ukraine)*
Fluctuation nanoclusters in liquid-like magnetics

39. V.O. Krasnov *(Lviv, Ukraine)*
Bose–Fermi–Hubbard model in the truncated Hilbert space limit

40. M. Krasnytska *(Lviv, Ukraine)*
Self-averaging on annealed networks

41. I. Kravtsiv *(Lviv, Ukraine)*
Soft-core fluid with competing interactions in contact with a hard wall

42. O. Krupnitska *(Lviv, Ukraine)*
High-field low-temperature properties of frustrated Heisenberg antiferromagnet on one-dimensional lattices

43. V. Kulinskii *(Odesa, Ukraine)*
Global isomorphism between molecular fluids and ising-like models: Yukawa fluid case

44. N. Lazarev *(Kharkiv, Ukraine)*
Density spectrum analysis of supercritical fluid

45. B. Lisnyi *(Lviv, Ukraine)*
Spin-1/2 Ising–Heisenberg distorted diamond chain with antiferromagnetic Ising and ferromagnetic Heisenberg interactions

46. M. Litniewski *(Warsaw, Poland)*
Effect of aggregation on adsorption phenomena

47. I.G. Marchenko *(Kharkiv, Ukraine)*
Temperature-abnormal diffusion in tilted periodical potentials

48. B.M. Markovych *(Lviv, Ukraine)*
A metal film on a dielectric substrate within jellium model

49. O.P. Matveev *(Lviv, Ukraine)*
Combining pump/probe PES and electronic Raman scattering to test for the thermalization of hot electrons

50. E.H. Megchiche *(Tizi-ouzou, Algeria)*
Determination of free energies of point defects by molecular dynamic simulation: Case of nickel

51. R. Melnyk *(Lviv, Ukraine)*
Van der Waals equation of state for hard-sphere system: A new twist to the old story

52. P. Müller *(Magdeburg, Germany)*
Thermodynamics of frustrated Heisenberg magnets on the kagome and pyrochlore lattices: Green's function approach and high-temperature expansion

53. I. Omelyan *(Lviv, Ukraine)*
On solving the moment master equations of population dynamics for spatially inhomogeneous systems

54. G. Panochko *(Lviv, Ukraine)*
Bose polaron in ideal Bose gas at finite temperature

55. A.S. Peletminskii *(Kharkiv, Ukraine)*
Equilibrium properties of a two-component Fermi gas coexisting with Bose-Einstein condensate of its heteronuclear bound states

56. V.M. Pergamenshchik *(Kyiv, Ukraine)*
Statistical model of a flexible inextensible polymer chain: the effect of kinetic energy

57. D. Portnyagin *(Lviv, Ukraine)*
Computational modeling of memory effects in turbulent flows

58. M. Pospíšil *(Praha, Czech Republic)*
Novel phase transitions in chemically heterogeneous slits

59. M. Pospíšil *(Praha, Czech Republic)*
Morphological and bridging transitions at nanopatterned walls

60. I. Ryzha *(Lviv, Ukraine)*
Fine-structure oscillations in catalytic carbon monoxide oxidation on platinum

61. P. Sarkanych *(Lviv, Ukraine)*
Ising model with invisible states on scale-free networks

62. D. Shapoval *(Lviv, Ukraine)*
Two-species reactive lattice gases on random catalytic chains: Annealed versus quenched disorder

63. Ya. Shchur *(Lviv, Ukraine)*
Porous silicon partly filled with water molecules: crystal structure, energy bands and optical properties from first principles

64. V. Shmotolokha *(Lviv, Ukraine)*
Generalization of the Van der Waals equation for anisotropic fluids in a disordered porous medium

65. M. Simončič *(Ljubljana, Slovenia)*
Hydrogen bonding between simple hydrides

66. V.M. Simulik *(Uzhgorod, Ukraine)*
Arbitrary spin and statistics in the new relativistic wave equation, example spin $s = 3/2$

67. G.A. Skorobagatko *(Lviv, Ukraine)*
Summation theorem and its application to exact non-eqiulibrium full counting statistics of tunnel current in quantum-point contacts

68. A. Sokolovsky *(Dnipro, Ukraine)*
A review of Bogolyubov method of the reduced description of nonequilibrium states

69. D. Stepaniuk *(Kharkiv, Ukraine)*
Microscopic environment of the D205 dye in $BmimBF_4$ in ground and excited states

70. R. Stetsiv *(Lviv, Ukraine)*
Low-frequency dynamics of one-dimensional systems with hydrogen bonds

71. M.Ya. Sushko *(Odesa, Ukraine)*
Recent developments in the theory of electrodynamic homogenization of random particulate systems

72. V. Tkachuk *(Lviv, Ukraine)*
Relation of entanglement of continuous variable graph states with graph properties

73. M. Tokarchuk *(Lviv, Ukraine)*
Generalized diffusion equation with fractional derivatives. Zubarev's NSO method

74. V.V. Tokarev *(Kharkiv, Ukraine)*
On applicability of rotational band approximation

75. A. Vdovych *(Lviv, Ukraine)*
Effect of hydrostatic pressure and longitudinal electric field on dielectric properties of CDP ferroelectric

76. O.V. Velychko *(Lviv, Ukraine)*
Dipole ordering and strain effects in the deformable Blume–Emery–Griffiths model

77. T. Verkholyak *(Lviv, Ukraine)*
Effect of the bond distortion in the Ising-Heisenberg model on the Shastry-Sutherland lattice

78. V. Vikhrenko *(Minsk, Belarus)*
Thermodynamic and structural properties of systems with SALR interaction on two- and three-dimensional lattices

79. V. Vikhrenko *(Minsk, Belarus)*
Monte Carlo simulation of a 3D solid electrolyte on a simple cubic lattice: concentration and electric field distribution at and without an external field

80. A.V. Vorobel *(Odesa, Ukraine)*
Combined effect of 1.5- and double scatterings on the Rayleigh line width near the vapor-liquid critical point

81. I.S. Vovchynskyi *(Kharkiv, Ukraine)*
Molecular dynamics simulation of 1-1'-spirobipyrrolidinium tetrafluoroborate acetonitrile solutions

82. V. Yanishevsky *(Lviv, Ukraine)*
Application of statistical physics methods to stochastic financial models

The 5th Conference

"Statistical Physics: Modern Trends and Applications"

Invited Lectures

Abstracts

3–6 July 2019, Lviv, Ukraine

Density functional theory for systems with competing interactions

A. Ciach

Institute of Physical Chemistry, Polish Academy of Sciences, 01-224 Warsaw, Poland

Density functional theory (DFT) for systems with competing interactions leading to self-assembly into clusters, networks or layers is constructed. The contribution to the grand thermodynamic potential associated with mesoscopic fluctuations is explicitly taken into account. The expression for this contribution is obtained by the methods known from the Brazovskii field theory. Physical interpretation of the fluctuation-contribution to the grand potential is discussed. A simplified theory valid for weakly ordered phases, i.e. for the high-T part of the phase diagram is verified by a comparison with the results of simulations. Simulation results for the short-range attraction long-range repulsion (SALR) interaction potential are presented, with a special focus no the effects of confinement.

A primer on quantum computing for condensed matter physicists

J.K. Freericks

Department of Physics, Georgetown University, Washington, DC 20057, USA

Quantum computing is exploding across the world. I will describe some of the successes along with some of the open challenges needed to make it an effective tool for advancing condensed matter theory. Quantum simulation requires three important steps: (1) state preparation; (ii) state evolution in time; and (iii) measurement of the quantities of interest. As an example, I will describe how digital computation can be employed to determine many-body Green's functions. Along the way, I will sketch some of the key issues one must confront in performing quantum computation and describe some of the critical open problems we still need to solve to enable exciting science to be performed on these machines. Current hardware cannot do anything too sophisticated, but if it continues to advance at a rapid pace, this will soon change. What are the most exciting condensed matter physics problems that can be solved with those next generation machines? Will we be ready to take advantage of these new capabilities?

Quantum spin liquid at finite temperatures

I. Rousochatzakis, S. Kourtis, J. Knolle, R. Moessner and N.B. Perkins

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Quantum spin liquids are long-range entangled states of matter with emergent gauge fields and fractionalized excitations. While candidate materials, such as the Kitaev honeycomb ruthenate α-$RuCl_3$, show magnetic order at low temperatures T, here I will present numerical simulations that demonstrate a dynamical crossover from magnon-like behavior at low T and frequencies ω to long-lived fractionalized fermionic quasiparticles at higher T and ω. This crossover is akin to the presence of spinon continua in quasi-1D spin chains, and will be shown to go hand in hand with persistent typicality down to very low T. This, which we argue is a signature of proximate spin liquidity and emergent gauge degrees of freedom more generally, will be useful for the numerical study of many finite-T properties of putative quantum spin liquids.

Dynamical Non-Equilibrium Molecular Dynamics

G. Ciccotti

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In the talk we will discuss the Dynamical approach to Non-Equilibrium Molecular Dynamics (D-NEMD), which extends stationary NEMD to time-dependent situations, be they responses or relaxations.

Based on the original Onsager regression hypothesis, implemented in the nineteen-seventies in computer simulation, the approach permits to separate the problem of dynamical evolution from the problem of sampling the initial condition.

D-NEMD provides the theoretical framework to compute time-dependent macroscopic dynamical behaviors by averaging on a large sample of non-equilibrium trajectories starting from an ensemble of initial conditions generated from a suitable (equilibrium or stationary non-equilibrium) distribution at time zero.

We discuss how to generate a large class of initial distributions. Indeed, the same approach applies to the calculation of the rate constants of activated processes and to the generation of hydrodynamic patterns (convective motion, relaxation of interfaces). The generality of the method will be illustrated by presenting applications to few key hydrodynamic processes (the "classical" flow under shear, the formation of convective cells and the relaxation of an interface between two immiscible liquids).

From the Ising model to sociophysics and back again — via the humanities: My adventures in a distant academic world

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Mine is an eclectic talk reflecting a variety of recent interests — all founded on the Ising model. I start with a discussion of the relationship between sociology and statistical physics and how the former inspired the latter 100 years ago. I discuss the "two cultures" and mutual distrust/misunderstanding between science and the humanities down the years, and the emergence of a third culture in the "century of complexity". After touching on the essence of network theory, I give three examples of applications to humanities: how fraudulent Scottish poetry was integral to the rise of nationalism, an ongoing debate about Vikings in Ireland and heroic epics of the East Slavs.

I discuss some of the joys and travails of bridging the academic cultural divide before returning to safe ground of the Ising model. I end with a scientometrics slant — how the third culture can generate impact. And how this type of "payback" is important for all cultures in a complex world.

Magnetic phase transition induced by an electric field

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Significant technological progress has been made recently in the electrical field control of magnetism, in particular electrical switching or reversal of magnetization or even tuning between phases. On the other hand theoretical papers have been mainly focused on the one-dimensional systems. In the present paper we have studied the influence of the interchain coupling, magnetic field, and next-nearest-neighbor interaction in the coupled XY spin chains model with the next-nearest-neighbor, Dzyaloshinskii-Moriya $(S_n^x S_{n+1}^y - S_n^y S_{n+1}^x)$, and magnetoelectric $(S_n^x S_{n+1}^y - S_n^y S_{n+1}^x) S_{n+2}^z$ interactions on the shape of the magnetization as a function of the electric field at finite temperature. Using the linear perturbation renormalization group recursion relations the phase diagram in the plane (temperature, electric field) is found. The phase transitions to two different low temperature phases and a reentrance behavior caused by the electric field are observed. At finite temperature for some range of the interchain interaction values in addition to changing the magnetization sign with reversal of the electric field, there is a possibility to the magnetization sign switch in finite electric field values with no applied magnetic field.

The physics of dendrimer-like DNAs: simulation and experiment

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Dendrimers are synthetic macromolecules, characterized by a highly branched and regular internal architecture. Recently, dendrimer-like DNAs (DL-DNAs) were synthesized via enzymatic ligation of Y-shaped DNA building blocks. These charged dendrimers represent a novel macromolecular aggregate, which holds high promise in bringing about targeted self-assembly of soft-matter systems in the bulk and at interfaces.

We present a joint simulational-experimental study of these novel macromolecules. Based on a bead-spring model for the DL-DNAs (of varying generation numbers) we perform large-scale simulations to determine the equilibrium properties and the conformational characteristics of these macromolecules. The obtained results are compared to light scattering experiments [1]. The simulation data provide a broad variety of additional information about the internal molecular structure of DL-DNAs by varying the generation number and the salinity of the solvent. In an effort to simulate concentrated solutions of DL-DNAs, we extract an effective, coarse-grained potential, based on Widom's particle-insertion method. With this potential at hand, we investigate the bulk behaviour of DL-DNAs. These findings are essential to investigate if these macromolecules are a viable candidate for the experimental realization of cluster crystals with multiple site occupancy in the bulk [2].

The study of these charged dendrimer systems represents a relevant field of research in the area of soft matter due to their potential role for various interdisciplinary applications, ranging from molecular cages for drug delivery to the development of dendrimer- and dendron-based ultra-thin films in the area of nanotechnology [3].

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The challenge of highly frustrated quantum magnets at finite temperatures

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Frustrated quantum spin systems are prominent and at the same time challenging quantum many-body models. The first challenge concerns the nature of the ground state that might be semi-classically ordered or magnetically disordered (valence-bond crystals, quantum spin-liquids etc.). The second challenge is given by the magnetization process of these systems, which may exhibit plateaus and jumps. Last but not least, the third challenge concerns their thermodynamic properties on which far less studies exist than for the ground state. Here we focus on the thermodynamics of highly frustrated quantum spin systems with flat excitation bands, in particular on frustrated bilayer [1] and kagome antiferromagnets [2]. The frustrated bilayer antiferromagnet is realized in $Ba_2CoSi_2O_6Cl_2$ [3] and the magnetization curve of this compound is characterized by well-pronounced plateaus and jumps. The specific flat-band physics allows a comprehensive description of the thermodynamic properties of $Ba_2CoSi_2O_6Cl_2$ and the prediction of a finite-temperature order-disorder transition in high magnetic fields [1]. For the kagome quantum antiferromagnet the description of low-temperature physics is particularly demanding, because there are several competing states on the low-energy scale. Based on large-scale finite-temperature Lanczos simulations we discuss the specific heat, the susceptibility as well as the magnetization process. We find a strong influence of frustration on thermodynamic properties not only at low but also at moderate temperatures. Moreover, we find indications for an ordered magnon-crystal phase slightly below the saturation field.

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Dynamical glass

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Classical many body interacting systems are typically chaotic (nonzero Lyapunov exponents) and their microcanonical dynamics ensures that time averages and phase space averages are identical (ergodic hypothesis). In proximity to an integrable limit the long- or short-range properties of the network of nonintegrable action space perturbations define the finite time relaxation properties of the system towards Gibbs equilibrium. I will focus on short range networks which lead to a dynamical glass (DG), using a classical Josephson junction chain in the limit of large energy densities or small Josephson energies. Close to these limits the Josephson coupling between the superconducting grains induces a short-range nonintegrable network in the corresponding action space. I will introduce a set of quantitative measures which lead to the Lyapunov time T_Λ, the ergodization time T_E, and to a diffusion constant D. In the DG the system fragments into large patches of nonresonant 'integrable' grains of size l separated by triplets of resonant chaotic patches, all surviving over large times. T_E sets the time scale for chaotic dynamics in the triplets. Contrary, $T_E \approx l^2/D$ is the much larger time scale of slow diffusion of chaotic triplets. The DG is a generic feature of weakly nonintegrable systems with a short range coupling network in action space, and expected to be related to nonergodic quantum metallic states of quantum-many-body systems in proximity to a many-body localization phase.

Computer simulations of liquids and solvation using density functional theory-based molecular dynamics: Liquid water

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The computer simulation of liquids and solvation using molecular dynamics methods is a powerful tool. Its applicability depends, however, on the accuracy and the time- and length-scales of the simulations. Whereas in "classical" molecular dynamics one applies parametrised force fields to describe the interaction between the atoms, in "ab initio" molecular dynamics (AIMD) one usually relies on density functional theory (DFT) with an approximation to the exchange-correlation term chosen to reproduce satisfactorily the properties of the system under investigation. Whereas the former allows large and long-duration simulations, the latter – called DFT-based MD (DFTb-MD) by us – is better suited in simulations where there is chemical (re)activity or an accurate force field is difficult to obtain for other reasons.

We have recently applied the DFTb-MD method to the study of various properties of liquid water. In particular we have gained knowledge of the importance of the van der Waals interactions, which were not described in the most common approximations of the XC term until recent years [1,2], We also describe the simulation of the melting temperature [3] and collective dynamics of water [4].

We further discuss the extension of AIMD toward quantum chemistry methods such as MP2 and the random phase approximation (RPA).

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Liquid-liquid transition in high pressure hydrogen by Quantum Monte Carlo methods

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We studied the transformation from molecular-insulating to monatomic-metallic fluid hydrogen upon increasing pressure, by first principle simulations based on both Density Functional Theory (DFT) and Quantum Monte Carlo (QMC) methods [1,2]. Below a critical temperature $T_c \in [1500\,\mathrm{K}, 3000\,\mathrm{K}]$, the transition is first order with a discontinuity in the specific volume, a sudden dissociation of the molecules and a discontinuous change in electronic properties like the momentum distribution and the electrical conductivity [3,4,5]. Above the critical point the transformation into the metallic dissociated state is continuous. Optical response of the system is obtained within the Kubo-Greenwood framework of DFT. Agreement with recent experimental results at NIF for reflectivity and absorption is observed. Our analysis suggest a coherent picture for apparently discordant experiments from different methods.

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Probing the non-Debye low-frequency excitations in glasses through fast quenching and random pinning

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It has been recently observed in numerical simulations that although they dominate the low-frequency spectrum, phonons are not the only low-energy excitations in glassy systems.

We show that, as temperature T decreases towards the dynamical crossover T_d, the low-energy spectrum is progressively populated by quasi-localized soft-modes whose density of states $D(\omega)$ follows a power law $\sim \omega^{s(T)}$ with $2 \leq s(T) \leq 4$. Considering the growing of s from Debye, i. e., $s = 2$, to non-Debye obtained by frozen randomly a fraction p of particles, we suggest that non-Debye sector results to be magnified by approaching the dynamical transition because of the presence of dynamical heterogeneous regions of linear size ξ.

Finally, we make an estimate of ξ s a function of T comparing the spectrum as temperature decreases with the spectrum as a function of p. Our result is compatible with a power law $\xi \sim (T - T_d)^{-\alpha}$ approaching T_d.

Modeling of field-controllable polymers for mechanical applications

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Field-controllable polymers define a class of applied materials exhibiting a strong coupling of mechanical and external fields. Typically, such polymers represent at least a two-component system: polymer matrix and functional moieties either embedded into the matrix or attached to it covalently. Although the external field acts only on functional moieties, its work is transformed to the polymer matrix due to mechanical coupling between the phases. Prominent examples of field-controllable polymers are (i) photo-deformable azopolymers which are able to transform light energy into mechanical stress and (ii) magneto-sensitive elastomers (MSEs). The latter are loaded with micron-sized iron particles and feature mechanical moduli that become strongly enhanced under magnetic field as well as the ability for magnetically induced deformations.

Obviously, both materials have a great potential for diverse actoric applications, e.g. serving as artificial muscles. For example, complex director fields imprinted into azo-containing liquid crystalline elastomers lead to sophisticated photomechanical response, resembling autonomous mechanical actions in living systems. Because of their unique properties, there is strong commercial interest to the applications of MSEs in numerous fields, from automotive to medicine. Prediction of mechanical properties is based on minimisation of the free energy which contains the elastic energy of the polymer matrix as well as the interaction energies of functional moieties with the field and each other. The application of external fields oft causes a considerable evolution of the local material structure. For azopolymers it is possible to predict time-dependent reorientation of the polymer backbones and appearance of the light-induced stress that dictates a direction of the macroscopic deformation.

In this presentation, a recent progress in the modeling of both field-controllable materials will be discussed. In particular, some examples how the local material structure defines the macroscopic properties and appropriate material models will be given.

Simple lattice model approaches in electrochemistry

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Lattice models like cellular automata approaches are interesting for modeling in a simple way complex non linear dynamic systems. This approach is versatile and has been used in a wide variety of domains like physics, biology, chemistry, urban traffic as well as trade markets. We apply such approach to domain of electrochemistry.

Here, the lattice sites represent chemical species in liquid or solid state. Reaction and diffusion can be modeled and the stochastic evolution of the system is set by rules which take into account the local environment and probabilities. These may depend on physical parameters like the electric potential. In some cases, the electric field spatial distribution can be dynamically modeled, by a simple analogy with a diffusion process. Electric field spatial distribution combined with reaction kinetics may result in complex morphologies exhibiting sometimes self-organised patterns or different roughness properties. We present applications of the approach in the domains of:

- aqueous corrosion;
- self-organised nanoporous structures by anodisation;
- electrodeposition.

In the different examples, characteristic morphologies are reproduced and correlations between morphologies, kinetics and electric field distribution highlighted.

Deep Reinforcement Learning: sometimes it works, more often it doesn't!

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"`AlphaGO`", the software that defeated a great Korean master at the game of Go in March 2016, is just the tip of a field of *artificial intelligence* (AI) called "Deep Reinforcement Learning". This theme is on the rise and is stirring up all kinds of fantasies. In this presentation, we will analyse the underlying principles of this discipline (Markov Decision Processes, Regression by Artificial Neural Networks) to better understand its possibilities, and above all, its limitations. And we will also see that we are desperately lacking theoretical tools to understand why algorithms sometimes produce prodigious results and why, in the same situation, the results can be catastrophic.

The 5th Conference

"Statistical Physics: Modern Trends and Applications"

Contributed Talks

Abstracts

3–6 July 2019, Lviv, Ukraine

Leopolis Scientifica: Scientific heritage versus modern trends in statistical physics

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Scientific heritage of Lviv is rather diverse including names, schools, traditions, buildings, and museums associated with various fields of science such as philosophy, astronomy, physics, mathematics, medicine, chemistry, biology, etc.

Keeping in mind the primary topics of Statphys 2019, namely: (i) modern trends and applications in statistical physics and (ii) the 110th anniversary of M.M. Bogolyubov, main attention of this contribution will be turned out to the names of Marian Smoluchowski and Department for Theoretical Physics of Lviv University, Stanislav Ulam and Lviv Polytechnic University, Stefan Banach and Lviv school of mathematics, as well as Ihor Yukhnovskii and Institute for Condensed Matter Physics.

Three-state mesoscopic model of a heterophase fluid in application to the dielectric-semiconductor transformations in expanded mercury

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The fluid states of mercury are described in the framework of a mesoscopic theory of a 3-phase random mixture of mutually transforming fluctuons. Fluctuons represent the mesoscopic liquid-like-metallic, liquid-like-nonmetallic, and gas-like species. Formulated free energy of the system of interacting fluctuons produces a thermodynamic equation of state. It is found that for an appropriate set of parameters both the vapor-liquid transformation and the metal-nonmetal transformation in the liquid phase of mercury are accurately described. This communication is mainly devoted to the dielectric-semiconductor transformation in mercury. It is shown that the observed dielectric anomaly in mercury is induced by an excitonic transition at the percolation threshold of the nonmetallic liquid fraction. The partial conductivities and dielectric permittivities of gas phase, as well as those of the semiconducting liquid phase are determined. Applicability criterion of the Landau–Zeldovich scenario of the gas-nonmetallic liquid transformation is formulated.

On the phase behavior of water-like fluids with square-well attractions and site-site association in slit-like pores. Density functional approach

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We study the adsorption and phase behavior of water-like fluid models with square-well inter-particle attraction and site-site association in slit-like pores by using a density functional theory. The models for water taken from [1] reproduce the bulk equation of state well [2]. The mean field theory and the first-order mean spherical approximation have been applied to account for the attractive interactions. The chemical association effects are taken into account by using the first-order thermodynamic perturbation theory. The influence of the slit-like pore width, the gas-solid interaction energy, and of the square-well width on the phase behavior have been explored [3]. A comparison with computer simulation data has been performed. Some results and perspectives concerning the adsorption of water-like models in a slit-like pore with walls modified by pre-adsorbed tethered chain molecules are presented. The presence of molecular brushes on the pore walls has important consequences for the behavior of water in pores [4].

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Universal equation of state for polymer solutions

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We reconsider the isothermal equation of state (EoS) for linear homopolymers in good solvents, $p = p(c, T)$, which relates the osmotic pressure, p, of polymers with the bulk concentration, c, and the temperature, T. The classical scaling theory predicts the EoS in dilute and semi-dilute regimes [1–2]. We suggest a generalized EoS which extends the universal behavior of polymer solutions up to the highly concentrated state and confirmed it by molecular dynamics simulations and using available experimental data. Our conjecture implies that properties of polymer chains dominate the EoS in the presence of many-body interactions. Our theoretical approach is based on a viral expansion in terms of concentration blobs leading to a superposition of two power laws in the regime of concentrated solutions [3].

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Bound magnon crystals of spin-1/2 Heisenberg diamond and octahedral chains as a statistical-mechanical monomer-dimer problem

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It has been recently verified that the lowest-energy eigenstates of the spin-1/2 Heisenberg diamond [1] and octahedral [2,3] chains follow in a highly-frustrated parameter region from flat bands, which correspond to magnons bound on vertical dimers of a diamond chain and square plaquettes of an octahedral chain, respectively. This fact allows a precise description of low-temperature thermodynamics above the monomer-dimer and monomer-tetramer ground states of the spin-1/2 Heisenberg diamond and octahedral chains from a mapping correspondence with a classical one-dimensional lattice-gas model of hard-core monomers.

In the present work we will adapt the localized-magnon approach to a less frustrated parameter region supporting more peculiar dimer-tetramer and tetramer-hexamer ground states of the spin-1/2 Heisenberg diamond and octahedral chains with a spontaneously broken symmetry. A direct comparison between the results stemming from the exact diagonalization and the developed localized-magnon approach implies that the low-temperature thermodynamics of the spin-1/2 Heisenberg diamond and octahedral chain above the dimer-tetramer and tetramer-hexamer ground states can be reformulated as a statistical-mechanical problem of hard-core monomers and dimers.

Acknowledgement: This work was supported by Slovak Research and Development Agency under the grant No. APVV-16-0186.

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From Bogoliubov to Majorana quasiparticles in topological superconductors

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In his seminal paper Bogoliubov has shown [1] that electrons bound (via effective pairing interactions) into the Cooper pairs are featured by the gaped quasiparticle excitations, comprising a superposition of the particle and hole contributions. This concept is nowadays getting a great deal of renewed interests because in topological materials such Bogoliubov quasiparticles can evolve into the Majorana-type objects, being identical to their own antiparticles. They are regarded as very promising candidates for quantum bits, because of their exotic (non-Abelian) statistical nature and protection against any perturbation [2].

Mutation from the Bogoliubov to Majorana quasiparticles can be realized in nanoscopic-size wires within two popular scenarios, relying either on: (i) the spin-momentum locking or (ii) the self-sustained helical magnetic order, both combined with the proximity-induced electron pairing [3]. We shall discuss the underlying microscopic mechanism responsible for topological superconductivity and present unique properties of the Majorana modes. We shall also give an overview of the experimental evidence for such quasiparticles localized at the boundaries of topologically nontrivial superconductors, and illustrate their robustness on internal defects [3] and leakage on the side-attached quantum impurities [4]. Finally, we will address recent signatures of the delocalized Majorana modes in two-dimensional structures.

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Zeros of partition function and observables

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It is worth noting that observation of the Lee-Yang zeros at the experiment is not a trivial task because of difficulties one faces in realization of a system with complex parameters. In the paper [1] the possibility of direct experimental observation of Lee-Yang zeros for partition function of spin system was found on the basis of analysis of decoherence of probe spin. Direct experimental observation of Lee-Yang zeros was reported in [2].

We study a two-time correlation function for probe spin-1/2 interacting with spin system and find relation of the correlation function with partition function of spin system in complex magnetic field. We conclude that measuring of time dependence of the correlation function allows direct experimental observation of Lee-Yang zeros [3].

Also, two-time correlation functions of a system of Bose particles are studied. We find that zeros of the correlation functions are related with the Lee-Yang zeros of partition function of the system. So, the zeros can be experimentally observed [4]. A particular case of Bose particles on two levels is studied in details. The zeros of two-time correlation functions and the zeros of partition function of the system are found and analyzed.

The obtained relations of the Lee-Yang zeros with zeros of correlation functions open additional possibilities for experimental observation and studies of the Lee-Yang zeros.

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Approximate statistical properties of quantum nuclei via Generalised Langevin Dynamics

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Nuclear quantum effects are relevant to describe processes of experimental significance occurring at low temperature or high pressure, and even surprisingly close to ambient conditions, as in the case of reactions involving proton transfer. The simulation of these effects still poses a formidable numerical challenge due to the exponential scaling of exact methods with the number of degrees of freedom. In spite of a considerable amount of work in this area, no general, affordable, method has emerged. In this talk, two recently developed schemes to compute static and time-dependent quantum nuclear properties will be presented. The first approach improves on the *ad hoc* Quantum Thermal Bath dynamics [1–3] by providing a systematic criterion to gauge zero point energy leakage, a well-know and often fatal limitation of the approach, and proposes an adaptive scheme to balance the leakage on-the-fly by enforcing the quantum fluctuation-dissipation theorem. The second approach provides an asymptotically exact method to sample the Wigner thermal density, a key quantity in semiclassical approximation of quantum time-correlation functions, using Langevin dynamics. The performance of both methods will be demonstated on model and realistic systems of increasing complexity.

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Surface free energy of a hard-sphere fluid at curved walls: deviations from Morphometric Thermodynamics

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We report molecular dynamics simulation results [1] for the surface free energy of hard-sphere fluid at cylindrical and spherical hard walls of different radii. The precision of the results is much higher than that in our previous study [Phys. Rev. E **86**, 060602 (2012)], allowing us to estimate the size of deviations from the predictions of Morphometric Thermodynamics (MT). We compare our results to the analytical expressions for the surface energy as a function of wall radius R and fluid density derived from the White Bear II variant of the Density Functional Theory, as well as to the leading terms of the virial expansion. For the cylindrical wall, we observe deviations from MT proportional to R^{-2} and R^{-3}, which are consistent with the available virial expressions. For the spherical wall, while the precision is not sufficient to detect statistically significant deviations from MT, the MD results indicate the range of densities for which the truncated virial expansions are applicable.

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Stress fluctuations, shear modulus and phase transitions

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In this presentation we shall review some recent progress and applications of the stress fluctuation formalism. In particular, we show how the shear stress relaxation modulus can be computed accurately in equilibrium molecular dynamics simulations [1]. Then we shall investigate the temperature dependence of the shear modulus, especially through the glass transition [2], in order to compare to predictions of the mode coupling theory, and experimental estimates. Last, we present recent results on linear viscoelasticity of a model glass former [3], in liquid and solid states, and discuss our results in terms of simple rheological models.

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Stochastic mechanism for improving selectivity of olfactory projection neurons

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Primary reception of odors happens in the olfactory receptor neurons (ORN). The ORNs synapse onto the mitral cells of olfactory bulb. These cells, known as bulbar projection neurons (PN), or secondary neurons convey odor signals to olfactory cortex. It is known that discriminating ability in PN is better than that in ORN. An established point of view is that better selectivity in PN is due to lateral inhibition. Lateral inhibition of PNs happens due to activity of inhibitory bulbar neurons. Recruitment of the inhibitory neurons takes place for high odor concentrations and decreases with decreasing concentration. Therefore, efficacy of lateral inhibition in improving selectivity of PNs should decrease for low concentrations. Such a decrease has been observed experimentally.

In this talk, another mechanism is proposed for selectivity gain in PNs, which is independent of lateral inhibition and could be as well efficient for low concentrations. This mechanism takes place for individual PN without involvement of other bulbar cells. The prerequisites of this mechanism are as follows: (i) the random nature of stimuli obtained by PN from ORNs, (ii) the threshold-type response of PN on those stimuli, (iii) the leakage in the PN's membrane. Similar mechanism is also possible in individual ORNs, as well as in "electronic nose" sensors based on adsorption-desorption of odors.

Here, as a PN model the neuronal model is used, which has been proposed before, [1]. Activity of single ORN is described as a Poisson process. As a result of detailed mathematical analysis it is concluded that PN's selectivity can be several tens times better than that of ORN due to the mechanism proposed.

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Basin entropy and testing for Wada basins to analyze the unpredictability of some physical systems

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In nonlinear dynamics, basins of attraction are defined as the set of points that, taken as initial conditions, lead the system to a specific attractor. This notion appears in a broad range of applications where multistability is present, which is a common situation in neuroscience, economy, astronomy, ecology, and other disciplines. Nonlinear systems often give rise to fractal boundaries in phase space, hindering predictability. When a single boundary separates three or more different basins of attraction, we call them Wada basins. Usually, Wada basins have been considered even more unpredictable than fractal basins. However, this particular unpredictability has not been fully unveiled until the introduction of the concept of basin entropy. The basin entropy provides a quantitative measure of how unpredictable a basin is. With the help of several paradigmatic dynamical systems, we illustrate how to identify the ingredients that hinder the prediction of the final state. The basin entropy together with two new tests of the Wada property have been applied to some physical systems such as experiments of chaotic scattering of cold atoms, models of shadows of binary black holes, and classical and relativistic chaotic scattering associated to the Hénon-Heiles Hamiltonian system in astrophysics.

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Self-averaging in the two-dimensional random-bond Ising model

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Effects of disorder on the properties of condensed systems are of great interest as a varying degree of impurities is present in every material studied in the laboratory. In some cases, disorder might lead to a loss of self-averaging, i.e., the behavior of a large sample with a specific realization of impurities will not be well described by the ensemble average normally calculated in an analytical or numerical approach. The question of (non)self-averaging is connected to the relevance of disorder answered by the Harris criterion (for pure systems with continuous phase transitions weak disorder is relevant only if the specific heat is divergent, i.e., the critical exponent $\alpha>0$). It was already shown that for pure systems with $\alpha<0$ the relative variance of thermodynamic observables of disordered counterparts weakly decreases as a power of system size L, indicating "weak self-averaging", while for the case with $\alpha>0$ this ratio approaches a non-zero constant as $L\to\infty$, indicating a lack of self-averaging. The most intriguing case is given by the two-dimensional Ising model, where $\alpha=0$. We study sample-to-sample fluctuations in a critical two-dimensional Ising model with quenched random bonds. Using replica calculations in the renormalization group framework we derive explicit expressions for the probability distribution function of the critical internal energy and for the specific heat fluctuations [1]. It is shown that the distribution of internal energies is Gaussian, the typical sample-to-sample fluctuations and the average value scale with L like $\sim L \ln\ln L$. In contrast, the specific heat is shown to be self-averaging with a distribution function that tends to a δ-peak in the thermodynamic limit $L\to\infty$.

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Systems with competing interactions under confinement

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Systems as different as mixtures of lipids in water, ternary mixtures containing surfactants, diblock copolymers, or colloidal systems with competing interactions have similar topology of the phase diagram. In all these systems the same liquid crystal phases are formed such as fcc cluster crystals, hexagonal, bicontinuous gyroid, or lamellar ones. When the liquid crystal phase is confined its structure at the boundary is deformed in a specific way depending on the orientation of the confining surface with respect to the unit cell of the liquid crystal phase. I will present the results describing the influence of confinement on a few different liquid crystal phases formed in mixtures of amphiphilic molecules and colloidal systems with competing interactions. The universal behavior of these systems will be emphasized.

Influence of interparticle correlations on electrophysical properties of solid electrolytes

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Solid electrolytes remain an area of intensive scientific activity due to their great potential in industrial applications like rechargeable batteries, fuel cells, supercapacitors, memory devices, etc. Their models can be considered as mobile charges of one kind in the presence of a compensating background.

A cumulant expansion with respect to renormalized Mayer functions is used for calculating the cell potentials of mean forces and constructing the free energy in the form of a density functional. In the lattice approximation, a system of equations is obtained for calculating the potentials of mean forces. The uncorrelated part of the electric field is accounted for through the Poisson equation. The short-range correlation effects are taken into account through the mean potentials. Correlations between particles are taken into account for the first neighbors only. In the case of sufficiently small electric fields, the distribution of the potential and charge is described by a linear differential equation of the fourth order. Depending on the ratio of the intensities of Coulomb and short-range Van-der-Vaals interactions, its solution shows damped oscillations with varying damping and oscillating constants.

In a more general case, with accounting of the correlations up to third neighbors and without restriction to weak fields numerical solutions for the charge and electric field distributions were obtained. Again, the concentration distribution showed an oscillating behavior. Moreover, the oscillating behavior of the charge distribution was observed without the external electric field at not too small mean charge concentration.

The project has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Sklodowska-Curie grant agreement No 73427 and the Ministry of Education of Belarus.

High spin cycles: Topping the spin record for a single molecule verging on quantum criticality

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Theory has predicted a number of interesting quantum critical points for one-dimensional magnetic systems. At such points the ground state and thus low-temperature properties of a material change drastically upon variation of an appropriate external parameter. Competing exchange interactions constitute one possibility to drive a magnetic system into criticality. But since one cannot design the size of exchange interactions at will, it remains open whether certain fascinating systems can ever be realized in the lab.

Here we report on the chemical synthesis of a mixed 3d/4f coordination cluster that turns out to be very close to a quantum critical point. It also shows a ground state spin of $S = 60$, one of the largest ever observed. $[Fe_{10}Gd_{10}(Me\text{-}tea)_{10}(Me\text{-}teaH)_{10}(NO_3)_{10}]\cdot 20MeCN$ ($Fe_{10}Gd_{10}$ in short) forms a nano-ring system of alternating gadolinium and iron ions with a nearest neighbour coupling and a frustrating next-nearest neighbour coupling between adjacent iron ions only. Such spin systems are termed delta (or saw-tooth) chains. They exhibit a variety of frustration effects, among them giant magnetization jumps as well as macroscopic degeneracies of the ground state with profound caloric consequences [1].

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Eigenstate thermalization for local and nonlocal operators

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The out-of-equilibrium behavior of quantum many-body systems is the subject of much recent interest. A fundamental question is the possibility of thermalization in isolation, i.e., in the absence of an external bath. Our current understanding of this issue is based on the eigenstate thermalization hypothesis (ETH). The ETH helps us reconcile unitary quantum dynamics with the predictions of statistical mechanics. I will introduce the ETH and then present scaling results for local and nonlocal operators.

Fidelity at Berezinskii–Kosterlitz–Thouless transitions

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This work aims to clarify a long-standing controversy concerning the behavior of the ground state fidelity in the vicinity of a quantum phase transition of the Berezinskii–Kosterlitz–Thouless type in one-dimensional systems. Contrary to the prediction based on the Gaussian approximation of the Luttinger liquid approach, it is shown that the fidelity susceptibility does not diverge at the transition, and numerical claims of its logarithmic divergence with the system size (or temperature) are explained by logarithmic corrections due to marginal operators.

Finite-momentum impurity in one-dimensional Bose gas

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Talking about impurities in condensed matter systems we mainly keep in mind the situation when a very small number of atoms is immersed in the majority of bath particles. In a linear approximation in density of these extraneous particles both effects of the impurity statistics and the impurity-impurity interaction can be freely neglected and one faces the problem of a single particle loaded in the many-body environment. When this medium is formed by cold Bose-condensed atoms the problem is usually called the Bose polaron one.

Recent experimental realization of single mobile impurities in Bose–Einstein condensates of alkalies stimulated theoretical efforts for studying the dynamic and spectral properties of Bose polarons which, however, are mostly directed on the investigation of low-energy parameters of the impurity spectrum and a question of the finite-momentum Bose polaron behavior is typically left opened.

In this talk we discuss the full momentum dependence of spectrum of a point-like impurity immersed in a dilute one-dimensional Bose gas. Particular we elaborate, the path-integral approach whose semi-classical approximation leads to the conventional mean-field treatment of the problem while quantum corrections can be easily accounted by standard loop expansion techniques. The extracted low-energy parameters of impurity spectrum, namely, the binding energy and the effective mass of particle, are shown to be in qualitative agreement with the results of quantum Monte Carlo simulations.

Ferromagnetism of $LaCoO_3$

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We theoretically study unconventional long-range ferromagnetic ordering in the film $LaCoO_3$ under tensile strain. According to the reported importance of the intermediate-spin (IS) excitations in $LaCoO_3$ with cubic structure [1,2], we argue that the experimentally-observed ferromagnetism in the strained compound [3,4] originates from the highly-fluctuative nature of high-spin (HS) states, which can be viewed as bi-excitons.

Employing *ab-initio* density-functional description followed by Wannier projection, strong-coupling, and exact-diagonalization approaches, we construct a series of approximations to account for crucial electron correlation effects responsible for HS fluctuations and magnetic exchange. The obtained amplitudes and spatial characteristics of magnetic couplings between the "dressed" HS states show a good agreement with experimental observations and provide important details to the physical picture of $LaCoO_3$.

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Mixtures of room temperature ionic liquids with molecular solvents: challenge for the molecular modelling techniques

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Room temperature ionic liquids (RTILs) have already found an impressive number of applications due to the versatility of their properties which are determined by their composition. In case of electrochemical application of the RTILs the diversity of credible systems can also be expanded by combining RTILs with dipolar aprotic solvents like acetonitrile (ACN), propylene carbonate (PC) and γ-butyrolactone (γ-BL). Many practically important macroscopic properties of these mixtures (such as conductivity, viscosity etc.) are modulated by structure and particle dynamics at microscopic level.

In this contribution we discuss how the results of experimental investigations of the set of imidazolium-based RTILs and their mixture with AN, PC and γ-BL by using conductometry, NMR and Raman spectroscopy and quasi-elastic neutron scattering (QENS) can be explained by utilizing quantum chemical calculations and molecular dynamics simulations [1–11]. Variation in microscopic structure as a function of mixture composition is addressed in terms of competition between inter-ion and ion-molecular interactions as well as the formation of weak H-bonds.

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Dynamic heterogeneities in undercooled metallic alloys: An ab initio molecular dynamics study

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Understanding evolutions of transport properties in undercooled liquids and their interplay with their structural features represents an important issue for solidification processes of metallic alloys, such as crystallization and formation of quasi-crystalline or amorphous phases [1–4]. In the present work, we focus on various classes of Aluminum alloys such as Al-Ni [5], Al-Cu [6], Al-Cr [7] and Al-Zn-Cr [8] that we investigated using ab initio molecular dynamics. We simulate the undercooling process of these alloys during which we monitor the structural and atomic transport properties. We find that diffusion, viscosity and structural relaxation time undergo a crossover between an Arrhenius and non-Arrhenius behavior at a temperature T_X during the slowing down, which corresponds to an onset of dynamic heterogeneities (DHs) that develop. The structural features display characteristics compatible with the occurrence of the icosahedral short-range order (ISRO) as well as the development of a medium range order (MRO) upon cooling. The interplay between the ISRO and MRO and the dynamic heterogeneities is examined. The differences and similarities between these alloys is also discussed.

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Ab-initio molecular dynamics study of the pressure dependence of the collective excitations in liquid Ga-Sb alloy

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Transverse and longitudinal dynamic structures of liquid equiatomic Ga-Sb alloy are computed from ab-initio molecular dynamics simulations. Thermodynamic states ranging from ambient pressure up to 10 GPa are considered, following the melting line.

The evolution of collective dynamic properties as a function of pressure is studied in connection with the topological and chemical order. We focus on the collective propagating modes from which sound speed and shear viscosity are deduced. The issue of a possible coupling between longitudinal and transverse modes is discussed. Special attention is paid to the evolution when undergoing the liquid-liquid transition at about 4 GPa [1].

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Interpolation scheme for accurate predictions of PMFs and dielectric constants of electrolyte solutions. The use in implicit solvent simulations

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We developed an interpolation method (i-PMF) for fast and accurate predictions of potentials of mean force (PMF) between univalent spherical ions interacting in explicit water [1]. The speed-up, compared to molecular dynamics simulations, is 10^5-fold. i-PMF can be used to estimate, for example, the strengths of salt bridges and the effects of bridging waters in simulations of biomolecules. We demonstrate that the method works for a variety of commonly employed water models, as well as for pairs of charged-uncharged and two uncharged solutes. In addition, we present similar interpolation strategy, called the i-EPS, for predicting the dielectric constant in aqueous electrolyte solutions as a function of ion size and solution concentration. i-EPS allows to predict accurate values that can be used in implicit simulations before needing explicit or experimental results.

We combine i-PMF and i-EPS to probe the association behavior of implicit ion simulations to model explicit electrolyte solutions. Cluster fingerprinting is explored in light of collective concentration dependent effects. Such approach is beneficial for studying large systems and to speed-up sampling: one needs accurate simulations of charged particles with the solvent averaged into the interactions between particles. The concentration dependence of the static permittivity for electrolyte solutions affects how particles interact and cluster, and we investigate what controls this dependency. We highlight the asymmetry of response with cation/anion particle size. The increased precessional freedom keeps the static permittivity somewhat higher about solvated anions than about solvated cations.

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Viscosity of the Inner Core

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The Earth solid inner core (IC), composed mostly by iron, is a highly attenuating medium. This property of the core is at odds with the widely accepted paradigm of the hexagonal close-packed (hcp) phase stability under the inner core conditions, because sound waves propagate through the hcp iron without energy dissipation. We show by first-principles molecular dynamics that the body-centered cubic (bcc) phase of iron, recently demonstrated to be thermodynamically stable under the IC conditions, is considerably less elastic than the hcp phase. Being a crystalline phase, the bcc iron possesses the viscosity close to that of a liquid iron. The attenuation of the inner core is due to the unique diffusion characteristic of the bcc phase. The liquid-like nature of the bcc phase at extreme pressures and temperatures allow to resolve a number of controversies and explain enigmatic features of the Core.

We thank VR (grants 2013-5767, 2014-4750, and 2017-03744), Scientific Research Foundation of Ningbo University (grant 421708130), Olle Engkvist Byggmästare Foundation, Swedish Government Strategic Research Area in Materials Science at LIU (grant SFO-MatLiU No. 2009 00971), and Spanish Ministry of Economy and Competitiveness (CGL2013-41860-P and CGL2017-86070-R) for financial support.

Correlation of clusters: partially truncated correlation functions and their decay

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Partially truncated correlation functions (PTCF) of infinite continuous systems of classical point particles with pair interaction are investigated. We derive Kirkwood–Salsburg (KS)-type equations for the PTCF and write the solutions of these equations as a sum of contributions labelled by certain special graphs (*forests*), the connected components of which are tree graphs. We generalize the method introduced by Minlos and Pogosyan [1] in the case of truncated correlations. These solutions make it possible to derive strong cluster properties for PTCF which were obtained earlier for lattice spin systems. The report is based on the article [2].

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Thermodynamics of the 2D $S = 1/2$ Shastry–Sutherland model and $SrCu_2(BO_3)_2$

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Reliable computation of the low-temperature thermodynamic properties of highly frustrated quantum magnets is on the one hand highly relevant for experiments, but on the other hand a considerable challenge since, e.g., conventional Quantum-Monte-Carlo (QMC) simulations suffer from a severe minus sign problem. $SrCu_2(BO_3)_2$ is famous for its rich physical properties and as a realization of the two-dimensional spin-1/2 Shastry–Sutherland model. Notwithstanding recent progress with QMC simulations in the dimer basis, the parameter regime relevant to $SrCu_2(BO_3)_2$ has remained inaccessible [1]. Here we present accurate results obtained from two other methods, namely Thermal Pure Quantum (TPQ) states and infinite Projected Entangled Pair States (iPEPS). We observe the emergence of a low-temperature peak in the specific heat C and relate it to the large number of bound states that emerge close to the first-order transition from the dimer to the plaquette phase.

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Quantum phase transitions and intermediate magnetization plateau of 1D Heisenberg spin systems

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According to the extended Lieb–Schultz–Mattis theorem, 1D periodic Heisenberg spin 1/2 systems with odd number of spins per unit cell have the gapless lowest energy excitation spectrum. This may leads to non analytical behavior of their ground state energy as a function of Peyerls distortions of the distances between neighbor unit cells (dimerization) and the appearance of spin-Peierls instability of the corresponding spin systems when they are coupled to three-dimensional phonons. The systems with even number of spin per unit cell usually have gapped energy spectrum and do not demonstrate spin-Peyerls instability.

We propose a special type of 1D spin systems with even number of spin per unit cells formed by weakly interacting segments of two different types. The first order of perturbation theory in the interaction between neighbor segments gives the gapless character of the lowest part of the energy spectrum. Using the density-matrix renormalization group method we studied numerically the dependence of spin-Peierls critical exponents for the ground-state energies of above systems on the value of the coupling between neighbor segments. Perturbative treatment also demonstrates the existence of gapped excitations which corresponds to the excitations inside the weakly interacting segments. This leads to the appearance of intermediate plateau in field dependence of magnetization at low temperatures. The stability of this plateau against the increase of coupling between segments and temperature is studied using the quantum Monte-Carlo method.

The authors acknowledge the support of the VolkswagenStiftung, Germany (via grant 151110)

Statistics of phase boundaries: renormalisation and sharp asymptotics

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Statistical properties of equilibrium systems under phase coexistence are influenced by the presence of phase boundaries. In two dimensions the latter are often well approximated by one-dimensional interfaces, whose distribution around the equilibrium Wulff shapes can be described to a high precision in the thermodynamic limit.

In this talk we present a general approach to studying such interfaces, which is based upon a finite-size renormalisation and suitable cluster expansions.

We illustrate the technique by deriving the sharp asymptotics for the distribution of magnetisation in the 2D low-temperature Ising model. We further present an example of an interface model, in which the analysis persists in the whole subcritical region.

Processes of creation and propagation of correlations in quantum many-particle systems

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We review some new approaches to the description of the evolution of states of many-particle quantum systems by means of the correlation operators.

Using the definition of marginal correlation operators within the framework of dynamics of correlations governed by the von Neumann hierarchy, we establish that a sequence of such operators is governed by the nonlinear quantum BBGKY hierarchy. The constructed nonperturbative solution of the Cauchy problem to this hierarchy of nonlinear evolution equations describes the processes of the creation and the propagation of correlations in many-particle quantum systems.

Furthermore, we consider the problem of the rigorous description of collective behavior of many-particle quantum systems by means of a one-particle (marginal) correlation operator that is a solution of the generalized quantum kinetic equation with initial correlations, in particular, correlations characterizing the condensed states of systems. In addition, we establish the mean field asymptotic behavior of the process of the propagation of initial correlations.

Thermal conductivity universality of disorder solids and complex crystals

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The behavior of the thermal conductivity of an amorphous substance, depending on temperature and pressure, is universal and does not depend on the details of the chemical structure of the substance. Polymers, structural glasses, metal glasses and biomaterials, as well as some complex crystal structures: orientation glasses, clathrate compounds, ferroelectrics, skutterudite, etc., have the same (similar) temperature dependence with characteristic pronounced features: low-temperature quadratic growth, "plateau" and the subsequent rise to the high-temperature limit. Within the framework of the phenomenon of hybridization of a low energy localized excitations with an acoustic excitations, a qualitative explanation is given of thermal conductivity universality. The hybridization of a manifold localized states with continuum acoustic modes is described by the well-known Fano–Anderson resonance.

Two-dimensional superlattices: from atomic planes to practical devices

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The superlattice is a regular structure with the period significantly larger than the typical distance between atoms, but smaller than the electron mean free path. A possibility to control the period and the symmetry of an artificial superlattice makes it an ideal playground for band structure engineering and designing materials with on-demand electronic properties. Recently, high quality two-dimensional superlattices have been obtained by stacking atomically thin materials, such as graphene. A range of ground-breaking experiments has followed this technological breakthrough, which includes reports on the emergence of superconductivity [1], the observation of the Hofstadter butterfly in the magnetic miniband structure [2] and the fractal quantum Hall effect [3].

Behaviour of a superlattice in strong perpendicular magnetic field is of particular interest as it allows experimental verification of important predictions of quantum mechanics, which can only be tested in real crystals at prohibitively high magnetic fields of the order of 10 kT. In this presentation I will review the electronic properties of two-dimensional materials and practical approaches for making superlattices with focus on my own recent experimental results.

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Quantum stabilization and phase transitions in quantum anharmonic crystals

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A theory of phase transitions in quantum anharmonic crystals is presented based on the use of path integrals. In this theory, phases of thermal equilibrium of the crystal are constructed as probability measures on spaces of continuous paths whereas the crystal itself is an infinite system of interacting anharmonic oscillators attached to the vertices of the d-dimensional simple cubic lattice. Correspondingly, a phase transition is understood as the existence of multiple phases at the same values of the external parameters, such as temperature etc. The relevant model parameters are: particle's mass m; interaction intensity J; rigidity R characterizing the spectrum of the Hamiltonian of a single oscillator. For a harmonic oscillator, R is merely Hook's law constant. Sufficient conditions are obtained and analyzed for the phase transition to occur at some temperature, respectively, not to occur at all temperatures. The latter effect – quantum stabilization, holds if $R > dJ$, which in the harmonic case is just the condition for the crystal to be stable. That is why, R is called effective quantum rigidity. It is shown that, in the case of double-well anharmonic potentials, R can be made as big as one wants by making m small (isotopic effect) or by applying sufficiently large external pressure.

Non-conserved magnetization, negative *g*-factors and 'fire-and-ice' spin configurations

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We examine general features of the non-commutativity of the magnetization operator and Hamiltonian for small quantum spin clusters. The source of this non-commutativity can be a difference in the Landé g-factors for different spins in the cluster, XY-anisotropy in the exchange interaction and the presence of the Dzyaloshinskii–Moriya term in the direction different from the direction of the magnetic field. As a result, zero-temperature magnetization curves for small spin clusters mimic those for the macroscopic systems with the band(s) of magnetic excitations, i.e. for the given eigenstate of the spin cluster the corresponding magnetic moment can be an explicit function of the external magnetic field yielding the non-constant (non-plateau) form of the magnetization curve within the given eigenstate. In addition, the XY-anisotropy makes the saturated magnetization (the eigenstate when all spins in cluster are aligned along the magnetic field) inaccessible for finite magnetic field magnitude (asymptotical saturation). We demonstrate all these features through three examples: spin-1/2 dimer, mixed spin-(1/2,1) dimer, spin-1/2 ring trimer. For the case when al least one of the unit cell spin in the lattice has negative g-factor the system can exhibit unusual frustration for ferromagnetic couplings leading to the ground states with ordered and disordered sublattice at the same time ('fire-and-ice'). We illustrate these features through the example of Ising–Heisenberg diamond chain with four different g-factors.

Density functional theory for nanoparticles at liquid-liquid interfaces

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We propose an extension of density functional approach to study the structure and thermodynamic properties of the system comprising a certain amount of nanoparticles at the interface between two partially miscible liquids. Model calculations have been carried out for a binary symmetric mixture of hard-sphere Yukawa fluids and for spherical, as well as for dimer nanoparticles. Despite simplicity, the model captures principal features of this type of systems. The results indicate that nanoparticles form layers and the number of the layers depends on the amount of nanoparticles and on their diameters. For the systems studied the formation of the layers evidences a strong localization of the nanoparticles at the interface. In the case of dimers we have also used the site superposition approximation to evaluate the angular-dependent density profiles

Fluid-mediated interactions between colloids in bulk and under confinement

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The behaviour of colloids can be effectively controlled by tuning the solvent-mediated interactions among them. An extensively studied example is the temperature-induced aggregation of colloids in the vicinity of solvent's criticality. In this talk, I will briefly describe the physics of such colloid-colloid interactions in bulk systems [1], and we will discuss how the interactions are modified int the presence of a surface and in confinement [2]. I will demonstrate strong *non-additivity* of solvent-mediated interactions and show how it affects the colloidal phase behaviour. I will also discuss the formation of capillary bridges between colloids and the accompanying bridging phase transitions [3]. In addition, I will describe an interface localization-delocalization transition, which may occur in a two-phase fluid confined into a slit, and will show how colloids can help to detect it [4].

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Information theory, machine learning and the renormalization group

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The connections between information theory, statistical physics and quantum field theory have been the focus of renewed attention. In particular, the renormalization group (RG) has been explored from this perspective. Recently, a variational algorithm employing machine learning techniques to identify the relevant degrees of freedom of a statistical system by maximizing an information-theoretic quantity, the real-space mutual information (RSMI), was proposed for real-space RG. Here we investigate analytically the RG coarse-graining procedure and the renormalized Hamiltonian, which the RSMI algorithm defines. By a combination of general arguments, exact calculations and toy models we show that the RSMI coarse-graining is optimal in a sense we define. In particular, a perfect RSMI coarse-graining generically does not increase the range of a short-ranged Hamiltonian, in any dimension. For the case of the 1D Ising model we perturbatively derive the dependence of the coefficients of the renormalized Hamiltonian on the real-space mutual information retained by a generic coarse-graining procedure. We also study the dependence of the optimal coarse-graining on the prior constraints on the number and type of coarse-grained variables.

Material design assisted by machine learning

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Efficient design and screening of the novel molecules is a major challenge in drug and material design. In this contribution we present a multi-stage pipeline in which several deep neural networks are used to generate and validate novel molecular structures with the desired properties. Here the Autoencoder network is trained on existing structures to convert discrete molecular representations to continuous vector representation and reconstruct back the structure for a given vector in that space. An Attention-based Sequence to Sequence model "spell-checks" errors in the generated structures, while a fully connected Regressor type network is trained to predict desired molecular descriptors. In addition, we extend the scheme by adding few steps assessing the quality of the generated molecules. To this end, we use oversampling techniques in the continuous space to generate candidate structures and compute Synthetic accessibility score to assess the likeliness of the molecule synthesis.

Towards the Heider balance — asymmetric social relations

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Removal of cognitive dissonance by classification of individuals as enemies or friends has been modeled with a set of differential equations (K. Kułakowski et al, IJMPC 16 (2005) 707). Under this dynamics, interpersonal relations tend to the structural balance, where the group is divided into two parts, mutually hostile but internally friendly. Here we generalize the model by releasing the condition on symmetry (reciprocity) of interpersonal relations. Sets of new stationary states are identified, consisting of at most four parts; four types of neighborhood of nodes in the network. Within each set, the states differ only in the numbers of actors of a given type of neighborhood. For each set, conditions of stability are specified. The results are interpreted within the Cooley theory of self-looking glass. In particular, a new index of self-acceptance is proposed. The results can be of interest for teachers and class tutors. More details in arXiv:1903.12464.

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Abstracts

3–6 July 2019, Lviv, Ukraine

Quantum Heisenberg antiferromagnet on frustrated bilayer lattices

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The $s = 1/2$ antiferromagnetic Heisenberg model on several bilayer lattices (square, honeycomb and triangular) with magnon states from the flat band with lowest energy in the presence of a strong magnetic field is considered. Due to the localized nature of the flat-band magnon states, these systems are mapped on the classical lattice gases of hard-core objects. Also, the standard strong-coupling perturbation theory is applied for constructing of the effective Hamiltonians. These effective models allowed to investigate the phase transitions related to the ordering of localized magnons. These phase transitions belong to the different classes of universality. For the antiferromagnetic model on a honeycomb bilayer lattice for a small deviations from the full frustration regime, a spin-flop transition, which occurs in a XXZ model with an easy axis of magnetization, was found. On the basis of an effective model, constructed in the case of square geometry, a theory for a magnetic compound $Ba_2CoSi_2O_6Cl_2$ in an external magnetic field for the description of its low-temperature properties is developed. The results of experiments for this compound have been reproduced and new predictions have been made, which require new experimental studies to confirm them.

Also, the ground state of the quantum Heisenberg antiferromagnet on the bilayers (square and honeycomb) in the absence of magnetic field is investigated. A variational approach has been applied for that. By comparing the variational energies, the ground-state phase diagrams are constructed. The obtained results are compared with the ones obtained recently by more sophisticated methods. Qualitative consistency and good quantitative agreement for some critical points are observed.

Electrical conductivity of suspensions of particles with thin electric double layers

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We present a theory accounting for the effect of the electric double layer (EDL) on the bulk electrical conductivity σ_{eff} of suspensions of nanosized particles. The theory is based on our recent results [1,2], obtained within the compact-group approach (CGA), for macroscopically homogeneous and isotropic 3D dispersions of hard-core–penetrable-shell spheres embedded in a continuous matrix. The shells are inhomogeneous and characterized by a radially symmetrical conductivity profile $\sigma_2(r)$. The rule of dominance for the overlapping constituents suggests that the local value of the conductivity in the system is determined by the distance from the point of interest to the center of the nearest particle. The desired σ_{eff} is shown to satisfy a certain integral relation that becomes rigorous in the quasistatic limit and is valid for the entire range of admissible volume concentrations c of the cores.

We apply this theory to suspensions of particles (cores) with thin EDLs (shells). In this case, the model profile $\sigma_2(r)$ is actually the conductivity distribution in the EDL surrounding an isolated particle and can, therefore, be estimated through the well-known Gouy–Chapman and Dukhin solutions to the Poisson–Boltzmann equation. Using such a model to process experimental data for suspensions of nanosized latex particles in aqueous KCl and HCl solutions of different molarities, we show its capability of recovering σ_{eff} in wide ranges of c.

We also discuss the uses of the model for estimating: the conductivity of the suspending liquid; the surface charge acquired by particles upon being dispersed into the base liquid; the parameters of their EDLs; the role of the ion mobilities near the interface; and that of the surface conductivity.

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One-dimensional *XY* model of magnetoelectric in the presence of an energy current

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The spin-1/2 *XY* chain model of magnetoelectric carrying an energy flux is studied using the Lagrange multiplier method [1]. The magnetoelectric coupling is described within the Katsura–Nagaosa–Balatsky mechanism [2]. Using the Jordan–Wigner transformation the problem is reduced to the Hamiltonian of free spinless fermions and can be solved exactly. We investigate the effect of the field λ driving the current of energy: the phase diagram in the (λ, magnetic field), (λ, electric field), and (magnetic field, electric field) planes are constructed and analysed at different model parameters.

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On the shape of invading population in oriented environments

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The properties of population spreading in environments with spatial anisotropy are analyzed within the frames of a lattice model of asymmetric (biased) random walkers. The expressions for the universal shape characteristics of the instantaneous configuration of population, such as asphericity A and prolateness S are found analytically and proved to be dependent only on the asymmetric transition probabilities in different directions. The model under consideration is shown to capture, in particular, the peculiarities of invasion in presence of an array of oriented tubes (fibers) in the environment.

Role of nonlocal interaction in theory of a weakly non-ideal Bose gas with condensate

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In this work, we perform a consistent analysis of quadratic approximation of the Bogoliubov model [1] for a weakly interacting Bose gas with condensate employing different model potentials. The equilibrium properties of the system are described by two coupled equations [2]: the first equation provides a relation between the total number of particles and chemical potential and the second one represents the minimum condition for the grand thermodynamic potential. We demonstrate that the coupled equations have no solutions for contact (local) interaction potential, although they formally reproduce the well-known results for the chemical potential and condensate density. Therefore, we consider some nonlocal model interaction potentials with nontrivial dependencies of their Fourier transforms in momentum space [3]. In the regimes close to experimental realizations with ultracold atoms, the contribution of the terms originating from the quadratic part of the truncated Hamiltonian to the chemical potential can be of the same order of magnitude as from its c-number part. Therefore, the spectrum of single-particle excitations in the quadratic approximation acquires a gap. The issue of the gap is also discussed.

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Direct calculation of surface free energy of mannitol by Molecular Dynamics simulations

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Surface Free Energy (SFE) is an important property of solid materials in numerous industrial applications ranging from nucleation [1] to powder flowability [2]. The calculation of this quantity through Molecular Dynamics simulations therefore becomes essential, since it allows to obtain the value of the SFE directly from its thermodynamic definition. Among the different methods developed to determine this quantity from computer simulations, the cleaving method [3] calculates the SFE directly in the reversible process that creates a surface (or an interface) from the bulk system while measuring the work done on the system during this process. In this work we show the extension of the cleaving method to a molecular system, the mannitol, which represents a first step towards the development of a multi-scale methodology which will make use of the cleaving method with coarse-graining to obtain the SFE for more complicated systems such as polymers.

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Shear stress correlations and collective excitations in liquid In via ab initio computer simulations

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A new direction in ab initio studies of condensed matter under pressure is focused on detection of liquid-liquid transitions in metallic liquids as well as on understanding of metal-nonmetal transitions in expanded liquids. Mainly static properties were studied across the liquid-liquid transformation in ab initio simulations, while practically very little information exists in the literature on features in the single-particle and collective dynamics across the transition.

We present an ab initio molecular dynamics study of liquid In within the pressure range from ambient one up to 10 GPa along the melting line. A model system of 300 particles was studied within density functional theory with electron-ion interaction represented by PAW potentials. Radial distribution functions, mean-square displacements, and velocity autocorrelation functions (VACF) are analyzed. The calculated frequency spectrum of VACF reveals two-peak structure, which evolves with pressure. Longitudinal and shear stress-stress autocorrelation functions were calculated from ab initio simulations and the dependence of shear and bulk moduli on pressure was estimated. Longitudinal (L) and transverse (T) collective excitations were observed in the shape of L- and T-current spectral functions. The L and T dispersion curves were estimated and analyzed for increasing pressure. We discuss the correspondence of peaks of frequency spectrum of VACF and flat regions in the obtained T-dispersion curves at different pressures.

Lattice-gas model of two-component fluid

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We consider a simple lattice-gas model of the two-component fluid with the Hamiltonian

$$H(\{n_i\}) = \sum_{i=1}^{V} \left(V_i^A n_i^A + V_i^B n_i^B \right) + \sum_{(ij)} \left(V_{ij}^{AA} n_i^A n_j^A + V_{ij}^{AB} n_i^A n_j^B + V_{ij}^{BA} n_i^B n_j^A + V_{ij}^{BB} n_i^B n_j^B \right), \quad (1)$$

where $n_i^A + n_i^B = \{0, 1\}$, the second sum runs over all lattice bonds denoted by (ij), and $V_{ij}^{AB} = V_{ij}^{BA}$. Using the Gibbs-Bogolyubov inequality [1], we obtain the following density functional for the grand potential:

$$\begin{aligned} &\Omega(T, \mu^A, \mu^B, V; \{\rho_i^A\}, \{\rho_i^B\}) \\ &= T \sum_{i=1}^{V} \left[\rho_i^A \ln \rho_i^A + \rho_i^B \ln \rho_i^B + (1 - \rho_i^A - \rho_i^B) \ln(1 - \rho_i^A - \rho_i^B) \right] \\ &\quad + \sum_{i=1}^{V} \left[(V_i^A - \mu^A) \rho_i^A + (V_i^B - \mu^B) \rho_i^B \right] \\ &\quad + \sum_{(ij)} \left(V_{ij}^{AA} \rho_i^A \rho_j^A + V_{ij}^{AB} \rho_i^A \rho_j^B + V_{ij}^{BA} \rho_i^B \rho_j^A + V_{ij}^{BB} \rho_i^B \rho_j^B \right). \end{aligned} \quad (2)$$

Moreover, $\Omega \equiv \Omega(T, \mu^A, \mu^B, V; \{\rho_i^A\}, \{\rho_i^B\})$ (2) must be minimized with respect to the local mean-field densities, i.e., ρ_i^A and ρ_i^B, $i = 1, \ldots, V$ satisfy the set of equations $\partial\Omega/\partial\rho_m^A = 0$, $\partial\Omega/\partial\rho_m^B = 0$.

We use this approach to discuss the liquid-vapor surface tension of the system at hand.

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Phase behavior of a cell fluid model with a modified Morse potential

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The influence of including the soft repulsion to the Morse interaction on the phase behavior of the cell fluid model is investigated. The calculation of the grand thermodynamic potential of the model is performed using the method of calculation proposed in [1]. It has been established that the presence of soft repulsion substantially expands the scope of the cell model to describe the first order phase transitions, particularly, in alkali metals. The connection of the values of the parameters of the modified potential of interaction with the coordinates of the critical point is shown, and the state equation is obtained in a wide range of temperatures and densities. It has been established that the potential of this type satisfactorily describes the gas-liquid phase transition. It also provides better agreement with the data of the experiment for the parameters of the critical point, as well as the liquid branch of the coexistence curves of sodium and potassium in comparison with the results obtained for the usual Morse potential [2].

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Critical behavior of a supercritical cell fluid

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The analytic method for the description of the critical behavior of the fluid system at temperatures above the critical value of T_c (in the supercritical region) is developed on the basis of a cell fluid model. The collective variables approach [1] is used. The role of the interaction potential is played by the Morse potential [2] possessing the Fourier transform. The behavior of a cell fluid model with allowance for non-Gaussian fluctuations of the order parameter is considered near the critical point in the formalism of the grand canonical ensemble. A calculation technique, elaborated in [3] for the grand partition function, thermodynamic potential and equation of state of the model within the framework of the simplest non-Gaussian quartic distribution, supplements the previous study based on the mean-field approximation. The latter is not valid in the close vicinity of the critical point.

The obtained nonlinear equation linking the average density and the chemical potential is investigated. Proceeding from the obtained equation of state, the curves describing the dependences of the pressure and isothermal compressibility on the density are presented for various values of the relative temperature [3]. The Widom line for a supercritical cell fluid is constructed taking into account the extreme values of the isothermal compressibility. A specific feature of the approach is to use exclusively microscopic characteristics of the model (parameters of the interaction potential) for obtaining macroscopic quantities (pressure and other macroscopic quantities). The developed approach can be applied to the description of a phase transition in simple liquid alkali metals.

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Influence of the correlated hopping on the X-ray photoemission spectra

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We present results of the investigation of X-ray photoemission spectra (XPS) for the strongly correlated electron system with both local and nonlocal correlations. We consider the Falicov–Kimball model with correlated hopping, the simplest model of strongly correlated electrons, extended by the inclusion of the interaction with deep core-hole state. Despite its simplicity, the Falicov–Kimball model has a metal-insulator transition for large Coulomb repulsion and is exactly solvable via dynamical mean-field theory in infinite dimensions. XPS response at finite temperatures is connected with the core-hole propagator which is exactly expressed by the functional determinants on the Keldysh contour in time domain.

The present study is a continuation of our previous works [1–2] which considered the effect of correlated hopping on thermal transport and optical spectra. As we found previously for a wide range of the correlated hopping parameters, there are some singularities on the single-particle density of states and on the transport function ("quasiparticle" scattering time). Due to these anomalies and violation of the electron-hole symmetry, there is a huge enhancement on the thermoelectric properties and the optical conductivity exhibits a number of interesting features in the vicinity of these singularities.

We show to what extent these anomalous features can be manifested on the X-ray photoemission spectra at finite temperatures.

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On Dobrushin's uniquess theorem

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We present a new, simplified proof of Dobrushin's uniqueness theorem for the case of a model with nearest-neighbour interactions. We use this theorem to prove the absence of a phase transition at arbitrary temperature of a model of continuous spins on a lattice with nearest-neighbour interactions and a convex local potential.

Ground states of a system of classical spins on an anisotropic triangular lattice and the spin-liquid problem in $NiGa_2S_4$ and $FeGa_2S_4$ compounds

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It is shown that the ground states of a system of classical spins on an anisotropic triangular lattice with interactions within an elementary triangular plaquette can be constructed by minimizing the energy of a single plaquette. Even in the case when all three angles between plaquette spins are different, there exist five global ground-state configurations with equal energies. The most complex of these is an incommensurate four-sublattice conical spiral structure. Our results may shed some new light on the experimentally observed spin-liquid-like disorder in $NiGa_2S_4$ and $FeGa_2S_4$ where a four-sublattice spin structure were observed.

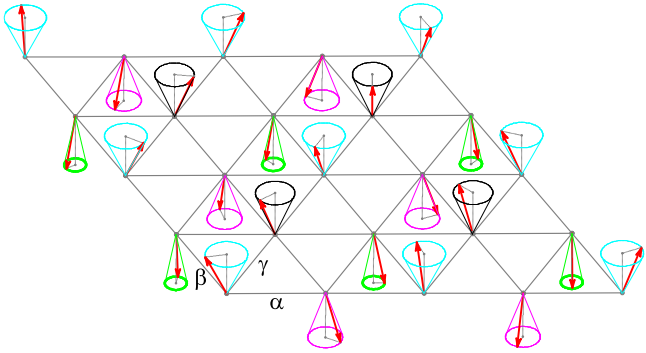

Figure 1: An example of four-sublattice spin configuration on an anisotropic triangular lattice. The angles between neighboring spins are equal to α, β, and γ. The cones for different sublattices are depicted in different colors. Within each sublattice, the spin structure is a simple spiral conical structure but on a triangular lattice with doubled lattice periods. The axes of all the cones are parallel.

An influence of an effective cation charge on the microscopic structure and solvation dynamics in non-aqueous media

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Rechargeable batteries based on lithium salts in low molecular weight solvents such as acetonitrile (AN), dimethyl sulfoxide (DMSO), γ-butyro-lactone (γ-BL) and propylene carbonate (PC) have become the dominating power source in the market of portable electronics. However, due to the safety problems of such batteries, the rarity and cost of lithium and the increasing energy intensity of the methods for extracting it from the earth's crust, great efforts have been devoted to finding and developing batteries containing other cations as an alternative. One of such non-Lithium candidates is Sodium and Magnesium. Therefore, an investigation of the microstructure and dynamic properties of these cations in non-aqueous solvents remains a relevant task. Molecular dynamics (MD) simulation is an effective tool to achieve this goal, but the problem of ion-molecular polarization especially within the first solvation shell (FSS) of a cation should be considered with a special attention.

With the aim to elucidate this problem, atomistic MD simulations of infinitely dilute solutions of Lithium, Magnesium and Sodium cations with variable charges in AN, DMSO, γ-BL, and PC were carried out by using MDNAES software package. The microstructure of the FSS of the cations was analyzed in terms of radial distribution functions, current coordination numbers and 3D structure of the FSS. Dynamics of cations' solvation was studied in terms of the self-diffusion coefficients and different kind of the time correlation functions. The results indicate the possibility of more accurate reproducing experimental data by variation of the effective cation charges.

Low temperature thermodynamics of one-dimensional exactly solvable spin models with impurities

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This work is devoted to the theoretical treatment of low temperature thermodynamics of some exactly solvable quantum models based on spin-1/2 XX-chain. We study analytically and numerically the finite spin-1/2 XX chains with defects of different nature: finite linear XX-chain with one distorted XX bond, finite linear XX-chain with one ZZ (or XX) impurity spin at one of the intermediate lattice site and two finite XX-chains, connected through an additional ZZ spin.

Real quasi-one-dimensional magnetic structures are characterized by different types of structure defects. The theoretical study of the influence of these defects on the energy spectrum and the thermodynamics of spin chains is of interest.

All above models can be reduced to the finite XX-chain with impurities. For these models we derived the analytical formulas for some principal and local thermodynamic characteristics and studied numerically their field and temperature dependence on the model parameters. In particular, we found a complex dependence of the heat capacity on applied magnetic field with numerous minima and maxima.

We found, that the field dependence of the magnetization at rather low temperatures has the finite jumps associated with impurity levels. In addition, the field dependence of average value of the ZZ impurity spin in the case of antiferromagnetic interaction with the main XX chain may have an oscillating behavior in a weak magnetic field and a jump in the critical field. We associate this jump with an impurity spin-flip along the direction of the magnetic field. So, the localized levels may effect noticeably on local thermodynamic characteristics.

E. Ezerskaya acknowledge the support from the VolkswagenStiftung, Germany (via grant 151110), and O. Dzhenzherov acknowledge the support from the State Fund of fundamental research of Modern Physics (via grant 33683).

Self-diffusion in the $BmimPF_6$/TfO-AN mixtures as seen by the quasi-elastic neutron scattering technique

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Motivated by their potential use as electrolytes in electrochemical applications, the mixtures of 1-buthyl-3-methylimidazolium hexafluorophosphate ($BmimPF_6$) and trifluoromethylsulfonate (BmimTfO), the commonly used ionic liquids (IL), with acetonitrile (AN) have been extensively studied by several experimental techniques in order to understand their macroscopic properties. Among the various direct experimental methods (i.e., those methods for which the space and time dimensions are comparable to the molecular dimensions and characteristic times of molecular processes, respectively), quasi-elastic neutron scattering (QENS) offers the most powerful techniques for analyzing ion and molecule dynamics in ion-molecular systems.

With the aim to elucidate the rotational and translational diffusive motions of $Bmim^+$ cation in $BmimPF_6$ and BmimTfO ILs and their solutions in acetonitrile-D_3, QENS measurements were carried out as a function of a temperature and composition. We used the MANTID software package for the QENS data reduction and analysis in the framework of the Bulavin–Ivanov model.

According to the obtained results, translational and rotational diffusion can be characterized at quantitative level for all the samples apart from pure ILs. It was found out that in binary mixture with a molar fraction of ILs more than 1%, translational diffusion is provided by individual and collective contributions. The contribution of collective motion increases with increasing temperature and molar fraction of IL. The variation of translational diffusion as a function of temperature follows Arrhenius equation. As the molar fraction of ionic liquids in the analyzed binary solutions increases, the translational motion of $Bmim^+$ cation slow down drastically and the activation energy of the process of translational diffusion of the cation increases several times, indicating a significant reinforcement of the inter-ionic association.

Models of economical process based on econophysics laws

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Econophysics is a science at the edge of economics and physics, it studies economic processes based on the use of fundamental laws of nature and physical theories. The use of econophysics allows to improve the research of economic processes.

The purpose of the research is to examine the application of basic physical models for building a macroeconomic model of Ukraine, which will allow making certain short-term forecasts for decision-making at the macro level.

As a result of applying econophysics basis, the macroeconomic model of the Ukrainian economy was constructed as a system of nonlinear differential equations. The entire population of Ukraine is divided into 7 main groups: population itself, workers of industrial enterprises, state employees, employees of the sphere of services, employees of raw materials enterprises, owners of enterprises, "elites". The distribution function of accumulation and income, demand function for essential goods and long-term goods are used. The equations for the accumulation of groups represent the balance of incomes and expenses for each group, the price of the product is determined from the balance of demand and supply on the market, the offer is the sum of imported and manufactured products within the country.

The stability of the system under Lyapunov, stationary states of the system was investigated. It is shown that the loss of stability of the solution of the system can be in the range of values close to the minimum purchasing power (bifurcation point).

In accordance with the economic situation in Ukraine, the parameters of the system of differential equations, which describes the macroeconomic model of Ukraine, are selected.

Classification of the equilibrium state of magnetic media with spin $s = 3/2$ and SU(4) symmetry of exchange interaction

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The equilibrium states of magnetic condensed media are classified on the basis of statistical mechanics [1]. The equilibrium states of such media are spontaneously broken with respect to magnetic SU(4) symmetry. In the Weyl basis, magnetic degrees of freedom are introduced, which include fifteen magnetic additive integrals of motion and the same magnetic order parameters. The quantum algebra of the Poisson brackets for the specified degrees of freedom is obtained. The conditions for the residual symmetry of equilibrium states for such media are formulated and the equations for the classification of magnetic order parameters are obtained. Its solutions are given in a number of special cases. As such cases, states that have a lower symmetry of the exchange interaction are considered. These include states with broken SO(3), SU(3), SU(2)xSU(2) symmetry. The admissible structure of the order parameters and the type of generators of unbroken symmetry are determined. An analysis of the similarities and differences of the new equilibrium states with the equilibrium states of magnets with spin $S = 1/2$ and $S = 3/2$ [2–4] is given.

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Time-dependent correlation functions of q-deformed Bose gas and Fisher zeros

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We find relation of time-dependent correlation function of q-deformed Bose gas with partition function depending on complex temperature [1]. Therefore, it is concluded that zeros of correlation function of q-deformed Bose gas are related with the Fisher zeros of partition function [2]. The complex temperature is caused by evolution of the system and q-deformation.

It is worth noting that the experimental observation of the Fisher zeros is not a simple problem because of difficulties with realization of a many-body system with complex parameters. The time-dependent correlation functions are experimentally observable quantities. So, the obtained relation opens new possibility to observe the Fisher zeros at the experiment.

The q-deformed algebra is associated with the deformed algebra leading to the minimal length [3]. Therefore the obtained result is also useful for studies of the Bose gas in quantum space.

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On the temperature evolution of a dissipative randomly driven system

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We investigate a kinetic equation for a dissipative system placed in a random field. It is assumed that the potential interaction in the system is small (small parameter λ). The dissipative interaction and the correlation functions of the random field are also assumed to be small and are estimated by one small parameter μ. A kinetic equation for the system under consideration up to the first order in λ and μ was obtained in [1] on the basis of the Bogolyubov reduced description method.

In our work the corresponding kinetic equation is obtained up to the second order of smallness in λ and μ. In fact, a generalization of the Landau–Vlasov kinetic equation to the systems under consideration is derived. A general nonlocal collision integral is obtained, and its local approximation is investigated in the case where the dissipation force between two particles is proportional to their veocity difference. In the absence of dissipation and an external field the kinetic equation coincides with the well-known Landau–Vlasov kinetic equation.

The evolution of a spatially uniform system is investigated. In order to solve the kinetic equation analytically, we consider the case where $\lambda \gg \mu$. In this situation the evolution of the system is described by the Landau–Vlasov kinetic equation with small corrections that are due to the dissipative and random forces. It is shown that after the mean free time the system is approximately described by the Maxwellian distribution function. Corrections to the Maxwellian distribution function are found on the basis of a generalized Chapman–Enskog method and evaluated with the help of a truncated Sonine polynomial expansion.

The corresponding time evolution equation for the temperature is derived, and it is shown that the spatially uniform system reaches a steady state. Corrections to the result [1] for the steady-state temperature of the system are obtained.

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Universal features of complex *n*-block copolymers

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The study is dedicated to the conformational properties of complex polymer macromolecules in form of n subsequently connected chains (blocks), that are characterized by different lengths and distinct chemical structure. For different solvent conditions, the inter- or intrachain interactions of some blocks may vanish, causing the rich conformational behavior. We pay attention mainly to the universal conformational properties of such molecules. The continuous chain model is used to describe the system and we apply the direct polymer renormalization group approach to derive the analytical expressions for the scaling exponent $\gamma(n)$, governing the number of possible conformations of n-block copolymer, and analyze the effective linear size measures of individual blocks. The numerical simulations of the simplest $n = 2$-block copolymer chain are performed as well for better illustration of the conformational behavior of such molecules.

Unification of thermo field kinetic and hydrodynamics approaches in the theory of dense quantum field systems

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We generalized the nonequilibrium thermo field dynamics in the framework of Zubarev's nonequilibrium statistical operator method [1] within the framework of Renyi statistics. The non-Markov transport equations in the thermo field presentation in Renyi statistics are obtained, which can be used to describe the nonequilibrium processes in quantum Bose and Fermi systems. In the case of $q \to 1$, when Renyi statistics are transformed into non-extensive Tsallis statistics, we obtain the corresponding generalized transport equations with non-additive entropy for the system. Based on this approach and Gibbs statistics, the generalized equations of the consistent description of kinetics and hydrodynamics for dense quantum field systems with strongly-bound states were obtained [2]. Using this approach, one can investigate both strong and weak nonequilibrium processes of nuclear matter, when the interaction between particles of the latter is characterized by strongly-bound states of an internucleon nature.

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Resummation of ε-expansion for co-polymer star exponents reveals the order of the phase transition in thermal denaturation of DNA

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In the mid-sixties of the last century Douglas Poland and Harold A. Sheraga suggested a theoretical model that describes the process of thermal denaturation of DNA in a manner analogous to phase transitions [1]. The model suggests that the order of the transition is identified by the value of a so-called "loop exponent" c. This is universal and can be expressed in terms of the exponents governing scaling properties of DNA strands. Their values, however, are not easily obtained and are usually identified through divergent (asymptotic at best) expansions. In this work we analyse applicability of resummed $\varepsilon = (4 - d)$-expansion for scaling exponents describing thermal denaturation of DNA in $d = 3$ dimensions. To this end, we used a fourth-order ε-expansion series for the co-polymer star exponents [2] and applied resummation techniques refined by the conformal mapping of a plane with a cut along the negative semiaxis onto a disc. The expressions take into account both properties of the solution and possible affects of self- and mutual interactions of single and double DNA strands. Subsequently, our results give evidnce of the fact that the effects studied significantly influence the strength of the first order transition. This becomes manifest in the changes shown by the scaling laws that govern the DNA loop and strand distribution.

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Thermodynamics of the $S = 1$ Heisenberg antiferromagnet on kagome lattice

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We discuss the thermodynamics of frustrated quantum Heisenberg antiferromagnets (HAFM) using high-temperature series [1] complemented by various interpolation schemes [2,3]. To be specific, we focus on the spin-1 kagome-lattice HAFM and examine the specific heat $c(T)$ and the uniform susceptibility $\chi(T)$ for this model. For the gapped ground state the energy values $e_0 = -1.369 \ldots -1.4416$ are reported and the gap is estimated as $\Delta = 0.17 \ldots 0.28$. We use the entropy method [2] and the $\log Z$ method [3] assuming the low-T behavior $c(T) \propto \exp(-\Delta/T)/T^2$. If we assume $e_0 = -1.43 \ldots -1.45$, various Padé approximants used for the interpolation yield almost the same temperature profiles $c(T)$ and $\chi(T)$. Moreover, the results using the entropy method agree well with those using the $\log Z$ method. The specific heat exhibits a shoulder-like behavior at low temperatures, i.e., starting from $T = 0$ it shows a fast increase to $c \approx 0.25$ until $T \approx 0.16$ which is followed by a slow increase to $c \approx 0.3$ as further increasing the temperature to $T \approx 1$, and the typical decrease to zero as $T \to \infty$. The entropy deficit estimated from the raw series [4] is noticeably smaller than the one for the spin-$\frac{1}{2}$ case thus giving some evidence for the absence of the low-T peak in $c(T)$ for the spin-1 kagome HAFM. The obtained $\chi(T)$ shows typical behavior growing to $\chi \approx 0.13$ at $T \approx 1$ and then following the Curie law as $T \to \infty$.

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Low-temperature peculiarities of thermodynamic quantities for decorated spin chains

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We discuss the origin of the peculiar low-temperature behavior of one-dimensional decorated spin systems [1–4] which was coined the pseudo-transition [5]. Tracing out the decorated parts results in the standard Ising-chain model with temperature-dependent parameters and an unexpected low-temperature behavior of thermodynamic quantities and correlations of the decorated spin chains can be tracked down to the critical point of the standard Ising-chain model at $\mathsf{H} = 0$ and $\mathsf{T} = 0$ [6].

We illustrate this perspective using as examples the spin-1/2 Ising-XYZ diamond chain and the coupled spin-electron double-tetrahedral chain. We have verified that the pseudo-critical exponents satisfy the following universality relation: $\alpha = \alpha' = \gamma = \gamma' = 3\nu = 3\nu' = 3$ [7].

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Fluid-fluid phase behaviour in the explicit hard spherocylinder solvent ionic model confined in a disordered porous medium

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We report our recent theoretical results on a study of the fluid-fluid phase transition of the explicit solvent model represented as a mixture of the restricted primitive model (RPM) of ionic fluid and neutral hard spherocylinders (HSC). We consider this model both in the bulk and in a disordered porous medium. To describe thermodynamic properties of such systems we combine two theoretical approaches, i.e., the scale particle theory (SPT) and the associative mean spherical approximation (AMSA) [1]. It is shown that the SPT is sufficient to provide a rather good description of a reference system taking into account hard-core interactions, and the AMSA is known to be efficient in treating the Coulomb interactions between the ions. Using the conditions of thermodynamic equilibrium, a phase coexistence for a RPM-HSC mixture is found at different temperatures, and the corresponding phase diagrams are built in the temperature-density and temperature-concentration planes. It is observed that the high-density phase mostly consists of the ions. On the other hand, the low-density phase is formed by a high concentration of solvent, thus the orientational order of HSC particles becomes possible in this phase. We have noticed that the orientation order strongly depends on the aspect ratio of HSC particles L_2/σ_2 and on the total pressure in the considered system. For instance, for $L_2/\sigma_2 = 5$ the low-density phase remains isotropic up to high pressures, while for $L_2/\sigma_2 = 10$ the formation of nematic phase of HSC particles is found at rather low pressures. In our study we discuss how a presence of disordered porous medium affects coexisting phases formed in RPM-HSC mixtures and establish conditions at which the nematic phase can occur in them.

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Two- and three-phase equilibria of polydisperse colloidal mixtures in bulk and random porous media

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We have studied the phase behavior of colloidal system, which is represented by polydisperse hard sphere Yukawa mixture in bulk [1] and random porous media [2] using extension and combination of high temperature approximation and scaled particle theory. The porous media are represented by the matrix of randomly placed hard-sphere obstacles. We have extended and applied the scheme developed to calculate the phase diagrams of polydisperse mixtures described by the truncatable free energy models, i.e., the models with Helmholtz free energy defined by the finite number of the moments of the species distribution function [3]. Due to the confinement, polydispersity effects are substantially enhanced [2]. At an intermediate degree of fluid polydispersity and low density of the matrix, we observe two-phase coexistence with two critical points, and cloud and shadow curves forming closed loops of ellipsoidal shape. With the increase of the matrix density and the constant degree of polydispersity, these two critical points merge and disappear, and at lower temperatures the system fractionates into three coexisting phases. A similar phase behavior was observed in the absence of the porous media caused, however, by the increase of the polydispersity [1,4].

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Nonequilibrium correlations in open quantum dynamics

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We study the memory effects and nonequilibrium correlations in open quantum systems, which was initiated recently in papers [1,2]. The nonequilibrium statistical operator method [3] was used to derive the non-Markovian master equation for an open quantum system, taking into account memory effects and the evolution of an additional "relevant" variable—the mean interaction energy of the composite system (the open quantum system plus its environment). This approach allows one to describe systematically the long-living nonequilibrium correlations associated with the total energy conservation. However, the price paid for this possibility is the need to solve the system of coupled evolution equations for the statistical operator of the open system and the additional nonequilibrium state parameters.

Our main concern is the time behaviour of the so-called quasi-temperature, which is a parameter conjugated to the mean interaction energy [1]. We derive the evolution equation for the quasi-temperature which has the form of the generalized thermodynamic relation envolving the generalized heat capacity [2]. Its right-hand side is nothing but the derivative of the total kinetic energy of the composite system.

Using this approach, we derive the system of kinetic equations for the generelized coherence in the dephasing model (which is known to be an exactly solvable one [4]) up to the second order in interaction taking into account the dynamical correlations in the "q-bit+environment" system.

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Aggregation and self-assembly of decorated nanoparticles by coarse-grained molecular dynamics simulations

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We consider a range of generic models for the nanoparticles decorated by ligands with the liquid crystalline groups, including the case of photosensitive mesogens.

In a melt, such nanoparticles are found to self-assemble predominantly into a glass-like polydomain lamellar morphology. For the case of chromophoric liquid crystalline groups (e.g. azobenzene), application of illumination with a suitable wavelength leads to cyclic trans-cis-trans photoisomerisation events. These aid effective transformation of a disordered or a polydomain glass-like state into a monodomain lamellar morphology. A range of properties such as: molecular asphericity, nematic and smectic order parameters, as well as clustering characteristics are analysed in a course of this photo-induced self-assembly [1].

In a solution under poor solvent conditions, nanoparticles aggregate into a nanogel network, due to strong liquid crystalline interactions between their ligands. The dynamics of network formation, as well as the final structure of the network, are found to depend strongly on a decoration pattern of nanoparticles. The cases of polar, planar patchy-like and uniform equatorial, as well an icosahedral patterns are considered. Network characteristics such as: the size and the dimensions of a largest subnetwork, average rank and local clustering coefficient, alongside with the effective elastic constant for the network are evaluated and discussed [2].

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Frustrated Heisenberg spin models defined on a kagome-lattice strip

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The quest for exotic quantum states in simple yet realistic spin models remains a challenge in the field of quantum magnetism. In this respect, the Heisenberg models defined on one-dimensional cuts from the kagome lattice (strips) represent intriguing spin systems exhibiting, as a rule, macroscopically degenerate classical ground sates. Using both large-spin semiclassical as well as exact-diagonalization numerical techniques, we analyze the quantum phase diagrams of uniform- and mixed-spin Heisenberg kagome strips containing five spins in the unit cell (S, $\sigma_i = \sigma$, $i = 1, 2, \cdots, 4$), which are placed on the central (S) and on the end (σ) sites of the unit-cell spin cluster. For the uniform-spin system ($S = \sigma = \frac{1}{2}$), we (i) re-examine the previously established phase diagram close to the boundary of the critical spin phase—i.e., the GS of a Heisenberg chain with an effective site spin $\frac{3}{2}$)—and (ii) extend the phase diagram by including the case of ferromagnetic nearest-neighbor $S - \sigma$ exchange bonds. For the mixed-spin $(S, \sigma) = (1, \frac{1}{2})$ system, we demonstrate that the critical spin-$\frac{3}{2}$ and spin-$\frac{5}{2}$ phases in the uniform case transform to Haldane-type gapped phases with effective site spins 1 and 3, respectively.

Support by Bulgarian Science Foundation (Grant DN0818/16) is gratefully acknowledged.

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Universal shape properties of mesoscopic polymer chains, polymer stars and their aggregates

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We analyse macromolecular shape by the dissipative particle dynamics simulations. In the **case study A** we discuss a single linear chain in a good solvent and examine its asphericity, prolateness, size ratio and their probability distributions. Good agreement is achieved with available theoretical and simulation results. In the **case study B** we extend our analysis to the single homo- and hetero-stars immersed in a solvent of variable quality [2]. Asphericity and related properties are examined at various arms compositions as the functions of solvent quality. For the homo-star, the asphericity maximum is found close to the θ-point condition explained by the interplay between the enthalpic and entropic contributions to the free energy. In the **case study C** we consider the changes in shape-related universal ratios for a homo-star and for its individual arms with the increase of the number of arms f. The results for the universal ratios show very good agreement with the available data from the Monte Carlo and molecular dynamics simulations [3], whereas some of the ratios are calculated for the first time. In the **case study D** we looked at the aggregation of the amphiphilic stars in a solvent [4]. Four architectures are examined: the miktoarm star, two different diblock stars and a set of four disjoint linear diblock copolymers. We observed four different shapes of aggregats: spherical, rod-like and disc-like micelles and a spherical vesicle. The change from a spherical to aspherical micelle shape is monotonous, whereas that from an aspherical micelle into a spherical vesicle is found to be discontinuous.

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Stepwise magnetization curves and bipartite entanglement of an exactly solvable spin-1/2 Ising–Heisenberg branched chain

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The spin-1/2 Ising-Heisenberg branched chain composed of a regularly alternating Ising spin and a couple of the Heisenberg spins, the former of which is laterally branched by the additional Ising spin, is rigorously solved in a presence of the external magnetic field. The exact solution is based on the transfer-matrix approach following a partial trace over degrees of freedom of the Heisenberg dimers. Within the framework of this rigorous method we have examined in detail the ground-state phase diagram, magnetization process and concurrence serving as a measure of bipartite entanglement. We have found four different ground states depending on a mutual interplay between the magnetic field, the Ising and Heisenberg coupling constants. Two ground states have character of the modulated quantum antiferromagnetic phase with a translationally broken symmetry, one ground state has character of the quantum ferrimagnetic phase, and the last ground state is the classical ferromagnetic phase. The three quantum ground states are manifested in zero-temperature magnetization curves as intermediate plateaux at zero and one-half of the saturation magnetization. The pair correlation functions and the concurrence are used to quantify the bipartite entanglement between the nearest-neighbor Heisenberg spin pairs, which are quantum-mechanically entangled in three quantum ground states either with or without spontaneously broken symmetry. The ground-state phase diagram and zero-temperature magnetization curves of the spin-1/2 Ising-Heisenberg branched chain are compared with the analogous results of the fully quantum spin-1/2 Heisenberg branched chain obtained within the density-matrix renormalization group calculations.

This work was financially supported by grant of The Ministry of Education, Science, Research and Sport of the Slovak Republic under Contract No. VEGA 1/0043/16 and by grant of the Slovak Research and Development Agency under Contract No. APVV-16-0186.

Global isomorphism between Buckingham and Yukawa fluids and lattice gas

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Global isomorphism is based on the idea of similarity of behavior of a simple fluid and lattice gas in entire liquid-vapor coexistence region. This "similarity" can be approximated by the projective map between the thermodynamic states of these systems.

$$n = n_* \frac{x}{1 + z\,t}, \quad T = T_* \frac{z\,t}{1 + z\,t}, \tag{1}$$

where (x, t) — describe state of lattice model. (T_*, n_*) — so called the parameters of the Zeno-element and represent the "limit" states of fluid system. We discuss their difference from commonly used Boyle temperature and density respectively.

We show how global isomorphism approach can be modified for the cases of the Buckingham:

$$\Phi_B(x;a) = \begin{cases} \infty\,, & x \le r_0/r_m, \\ \frac{\varepsilon}{1-6/a}\left(\frac{6}{a}\,\exp\left(a\left(1-x\right)\right) - \frac{C}{x^6}\right), & x > r_0/r_m\,, \end{cases} \tag{2}$$

and the hard-core attractive Yukawa:

$$\Phi_Y(r;\gamma) = \varepsilon\,\frac{\exp\left(-\gamma\left(r-\sigma\right)\right)}{r} \quad r > \sigma \tag{3}$$

potentials using the idea of homogeneity transformation within the potentials of Mie-class. This modification allows to describe the critical parameters for Buckingham potential and check the agreement with numerical data. We check a number of linear relations which are simple consequences of (1), among them the relation of the critical point line:

$$\frac{2\,n_c}{n_*} + \frac{T_c}{T_*} = 1 \tag{4}$$

Violation of this condition makes it possible to predict the disappearance of the liquid binodal branch,when the potential (3) becomes too short-ranged.

Modeling of noise effect on self-similar mode of ice surface softening during friction

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Softening of ice surface under friction is explored in terms of the rheological model for viscoelastic matter approximation. The nonlinear relaxation of strain and fractional feedbacks are allowed. Additive non-correlated noise associated with shear strain, stress as well as with temperature of ice surface layer, is introduced, and a phase diagram is built where the noises intensities of the stress and temperature define the domains of crystalline ice, softened ice, and two types of their mixture (stick-slip friction). Conditions are revealed under which crystalline ice and stick-slip friction proceed in the self-similar mode. Corresponding strain power-law distribution is provided by temperature fluctuations that is much larger than noise intensities of strain and stress. This behavior is fixed by homogenous probability density in which characteristic strain scale is absent. Since the power-type distribution is observed at minor strains it meets self-similar rubbing mode of crystalline ice surface. An analysis of the time dependences of friction force was carried out by using a fast Fourier transform. Fluctuations are detected with the spectral power density of the signal, which is inversely proportional to the frequency and demonstrates the realization of $1/\omega^{\alpha}, 0 < \alpha < 2$ or "pink" noise. It was found that the behavior of the spectrum is related to the course of the prehistory of nonequilibrium rubbing process. Research of autocorrelation function form of random fluctuations of friction force allowed to reveal the frequency characteristics of rubbing. The presence of weak correlation is shown. The obtained results reflect the real frictional conditions and can be used for predicting the rubbing force value or ice surface states (phases) during a certain correlation time. Thus, it is possible to establish the necessary external conditions to achieve the desired stable ice friction mode.

Collective scattering of gas stream by impurity clusters: wake-mediated interaction, post-soliton structures and disorder-enhanced shock waves

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We show specific effects of collective scattering for a cloud of heavy impurities (a cluster) exposed to Langmuir-gas stream. Formation is presented of a common density perturbation and shock waves, both being generated collectively by a system of scatterers at sudden application of the stream-inducing external field. Our results demonstrate that (i) the scattering of gas stream can be essentially amplified, due to nonlinear collective effects, upon fragmentation of a solid obstacle into a cluster of impurities (heterogeneously fractured obstacle); (ii) a cluster of disordered impurities can produce considerably stronger scattering accompanied by enhanced and accelerated shock wave, as compared to a regularly ordered cluster. We also show that the final steady-state density distribution is formed as a residual perturbation left after the shock front passage (a post-soliton structure). In particular, a kink-like steady distribution profile can be formed as a result of shock front stopping effect. The possibility of the onset of solitary diffusive density-waves, reminiscent of avalanche (or precursor-solitons), is shown. Specific properties of non-Newtonian induced dissipative interaction and its asymptotic behavior are discussed.

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Public transportation networks as complex systems: between data processing and statistical physics

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In this study, we present quantitative analysis of some public transportation networks (PTN) viewed as complex systems [1]. We apply a multi-disciplinary approach integrating methods in both data processing and statistical physics [2] to investigate the correlation between PTN topological features and their operational stability.

Initially, to present a PTN in the form of a complex network (i.e. a graph consisting of vertices-nodes and edges-links), we perform a coarse-graining procedure to merge stations considered to be within a reasonable walking distance (e.g. stops across the street) by implementing a DBSCAN clustering algorithm to the transport dataset.

Subsequently, we analyse the topological features of the resulting complex networks calculated for various network representations reflecting PTN operational features. In the second part of our analysis we assess the vulnerability of PTN by generalising the percolation scenario and removing network constituents according to different protocols (attack scenarios). We observe correlations between network topological features and its stability with respect to random failures and targeted attacks.

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Diffusion of hard sphere fluids in a disordered porous media from generalized Enskog theory

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We present a generalization of the Enskog kinetic theory for hard sphere fluids in a disordered porous media. In this approach the properties of considered model are defined by the contact values of fluid-matrix and fluid-fluid pair distribution functions. In this report the corresponded contact values of pair distribution functions are obtained from the scaled particle theory. The developed theory is applied for the investigation of the diffusion of hard sphere fluids in a disordered porous media for two types of porous media, namely for a hard-sphere matrix and for an overlapping hard-sphere matrix. The effects of fluids density, matrix porosity and morphology, fluid to matrix sphere size ratio on the self-diffusion coefficient are illustrated. Some comparison with computer simulations data is presented. The obtained results are generalize for the mixture of hard sphere fluids in a disordered porous media and corresponded self-diffusion coefficients are studied in dependence from the size ratio of different fluid species.

Fluctuation nanoclusters in liquid-like magnetics

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Problem of finite-size magnetic nanoclusters formation in an infinite system near phase transition point is formulated on the base of the Ising-like Hamiltonian and the lattice-gas model [1,2]. The only short-range interparticle interactions within the cluster and with the external environment are taken into account. The effective formula for number for nearest neighbours in surface layer of spherical nanocluster is derived. The Grand thermodynamic potential of the investigated system is calculated in the self-consistent field approximation.

The set of differential equations for parameters: concentration, magnetization, radius of the nanocluster are solved exactly. It was shown the appearance of certain point (below and upper of global ferroelectric phase transition temperature) at which a different types of nanoclusters arise. Normal low for size distribution of nanoclusters takes into account a chaotic character of order parameter fluctuations in the infinite system. The nanocluster mean size, their magnetic moment and the conditions of stability with changes in temperature are discussed.

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Bose–Fermi–Hubbard model in the truncated Hilbert space limit

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We investigate the phase transitions in the Bose–Fermi–Hubbard model proposed for description of thermodynamics and energy spectrum of the ultracold mixtures of Bose- and Fermi-atoms in optical lattices. The study of the fermion subsystem influence on the phase transition (PT) from the normal (Mott insulator, MI) phase to the superfluid (SF) one with the Bose-Einstein condensate is our main task. Consideration is performed for the case of infinitely small fermion transfer in the limit of truncated basis of the single-site states of bosons ($n_i \leq 1$ for hard-core bosons, and $n_i \leq 2$). The boson-fermion interaction U' is taken into account exactly while the hopping t_0 of bosons is considered within the mean-field approximation.

The regime of fixed values of chemical potentials (μ and μ', respectively) of Bose- and Fermi-particles is the basic one in our study. Analyzing the behavior of the BE condensate order parameter and the grand canonical potential, we have built the (μ, μ'), (μ, t_0) and (μ, T) phase diagrams at $T = 0$ and at the nonzero temperatures. It is shown: i) in the cases when transition to the SF phase is accompanied by the change of mean number of fermions, the PT order changes from the 2nd to the 1st one; this result corresponds to the literature data (DMRG calculations for harmonic trap); ii) at non-zero temperatures, the re-entrant transitions (when the SF phase is an intermediate one) can exist; iii) there are two types of SF phase that differ by fermion concentration; iiii) the shape of the MI phase regions (so-called lobes) in the (μ, t_0) diagrams and the localization of the 1st order PT segments on them depend on the μ' level position.

Using the fermion-hole transformation, a correspondence between cases of the B-F on-site repulsion and attraction is established. Based on the phase diagrams, built within the framework of the grand canonical ensemble, the conditions of the SF phase existence at $U' > 0$ and $U' < 0$ are analyzed. The diagrams (U', t_0), that illustrate the difference of behaviour of the BF mixture in these cases, are obtained. A relation to available experiments data is discussed.

Self-averaging on annealed networks

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Self-averaging (SA) is a basic concept for systems with quenched randomness. In experiments, SA is realized by averaging over a sufficiently large sample. In theoretical description and numerical simulations, a physical property of a system is said to be SA if the relative variance of its value averaged over all disorder realisations tends to zero with an increase of systems size.

An annealed network is defined as an ensemble of all networks consisting of N nodes assigned to a given degree sequence $\{k\} = (k_1, ..., k_N)$ [1]. The linkage between nodes is taken to fluctuate for each fixed sequence, each particular linkage configuration being a realization of an annealed structural disorder. The prominent feature of an annealed network is that the partition function $\mathcal{Z}(\{k\})$ calculated for given degree sequence $\{k\}$ by averaging over random linkage does not depend on a particular choice of $\{k\}$: $\mathcal{Z}(\{k\}) = \mathcal{Z}$. This means that the free energy is a self-averaged quantity too.

In our analysis, we consider a generalized Ising model with random spin length on an annealed scale-free network and show that its free energy is a SA quantity too. We present an asymptotic analysis [2] of its thermodynamics and show that the model is characterized by a rich phase diagram with a variety of phase transitions in four different universality classes [3]. We discuss possible applications of the model considered.

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Soft-core fluid with competing interactions in contact with a hard wall

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Fluids with a pair potential characterized by short-range attraction and long-range repulsion (SALR potential) have been intensively studied for more than a decade and still remain of great interest due to their unusual phase behavior and specific structure properties [1,2]. A SALR potential is of coarse-grained nature and can be used to effectively describe a solvent-mediated interaction between various complex molecules or colloidal particles, such as star-polymers, proteins, grafted nanoparticles, etc. A number of models and corresponding theoretical approaches have been proposed to predict structural and thermodynamic properties of such fluids. However, in most of them the core of fluid particles was considered as strongly repulsive. In our study we focus on a fluid with an interaction, which combines soft core and SALR potentials by representing them in the form of the three-Yukawa potential. The results of Monte Carlo simulations obtained by us show that such a model exhibits microphase separation and clustering phenomena similar to that observed in other SALR models. Moreover, we have noticed that in the case of a fluid confined between two hard walls these phenomena become even more pronounced, e.g. the cluster formation in the confinement can occur at temperatures higher than in the bulk. To understand the effect of confinement in such systems, we aim to develop a field theory approach enabling us to describe a three-Yukawa fluid near a hard wall. As the first step we apply the formalism previously proposed by us for a two-Yukawa fluid [3] and extend it to the case of a three-Yukawa model. At this stage of theory development we restrict our study to the region beyond the cluster formation and verify reliability of our theoretical approach under moderate conditions.

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High-field low-temperature properties of frustrated Heisenberg antiferromagnet on one-dimensional lattices

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We consider the spin-1/2 antiferromagnetic Heisenberg model on several one-dimensional frustrated lattices (double-tetrahedral chain [1], octahedral chain [2] and triangular tube [1]) with almost dispersionless (flat) lowest magnon band in a strong magnetic field. If the band is strictly flat, the thermodynamics of the model can be studied in detail in the low-temperature high-field regime after mapping the problem onto classical hard-core lattice-gas models. The aim of our study is to develop a systematic theory of the low-temperature high-field properties of the considered chains using the concept of localized magnons [3,4]. For this purpose we construct the low-energy effective Hamiltonians using the standard strong-coupling perturbation theory. To analyze the region of the applicability of the obtained effective Hamiltonians we perform extensive exact diagonalization and density matrix renormalization group calculations and compare them with the results for the initial models. We examine the constructed effective models to explain properties of the frustrated quantum Heisenberg antiferromagnets in the regime of high magnetic fields and low temperatures with special focus on the magnetization and the specific heat.

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Global isomorphism between molecular fluids and ising-like models: Yukawa fluid case

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Zeno-line and asymmetry effects of liquid-vapor equilibrium for molecular fluids are considered within the global isomorphism with the Ising-like models. The latter is based on the geometric reformulation of the (approximate) linearities of the density binodal diameter (the rectilinear diameter law) and the unit compressibility line (the Zeno-line). The correspondence takes the form of projective mapping between thermodynamic states of a fluid characterized by density n and temperature T and the Ising-like (lattice gas) model with density x and temperature t variables correspondingly:

$$T = T_* \frac{z\,\tilde{t}}{1 + z\,\tilde{t}}, \quad n = n_* \frac{x}{1 + z\,\tilde{t}}, \quad \tilde{t} = t/t_c \tag{1}$$

We demonstrate how the parameters n_* and T_* of the transformation (1) depend on the screening parameter λ of the potential:

$$\Phi_{HCYF}(r) = \begin{cases} -\Phi_0 \frac{e^{-\lambda\, r/\sigma}}{r/\sigma}, & \text{if } r > \sigma \\ +\infty, & \text{if } r \le \sigma. \end{cases}$$

of hard core Yukawa fluid (HCYF) class of systems. These parameters determine the critical point locus. Based on simulation data we show that besides the rectilinear diameter law HCYF demonstrates some other linearities which follow from Eq. (1). In particular we construct the critical point line in reduced variables $(T_c/T_*, n_c/n_*)$. The drastic difference in behavior of $n_*(\lambda)$ and standard Boyle-related parameter $n_B(\lambda)$ of the Zeno-line leads to the theoretical value λ_* above which the liquid branch of the binodal lose its stability. The results are compared to those of computer simulations. The peculiar linear correlation between n_c and $1/T_c$ first observed in simulations of Y. Duda et al. is obtained on the basis of projective isomorphism relations (1) for not too short-ranged potentials ($\lambda < 6$) where the stability of liquid phase takes place.

Density spectrum analysis of supercritical fluid

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The fluctuations of fluid density beyond the critical point can be very large due to diverging compressibility. Molecular dynamics (MD) simulation shows that the distribution function of these fluctuations differs from Gaussian, which indicates that the fluid is heterogeneous. We describe a general approach to analyze the density spectra, which reduces the problem to the solution of an integral equation. The nth-nearest-neighbor distribution functions in a uniform system are applied as base functions. The high-accuracy MD data of simulated argon are used to demonstrate the performance of the proposed method.

Spin-1/2 Ising–Heisenberg distorted diamond chain with antiferromagnetic Ising and ferromagnetic Heisenberg interactions

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The spin-1/2 Ising–Heisenberg model on a distorted diamond chain is exactly solved by the transfer-matrix method. In case of antiferromagnetic Ising and ferromagnetic XXZ Heisenberg interactions an influence of the quantum fluctuation and the parallelogram distortion on the ground state, magnetization, susceptibility and specific heat are investigated in detail. It is demonstrated that the zero-temperature magnetization curve may involve intermediate plateaus just at zero and 1/3 of the saturation magnetization. The temperature dependence of the specific heat shows up to four distinct peaks at zero magnetic field and up to five distinct peaks at a weak magnetic field. The physical origin of all observed additional peaks of the specific heat has been clarified on the grounds of dominating thermal excitations. The low-temperature two-peak thermal behavior of the specific heat is comprehensively studied.

Effect of aggregation on adsorption phenomena

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Adsorption at an attractive surface in a system with particles self-assembling into small clusters is studied by Molecular dynamics (MD) simulation. We assume Lennard-Jones plus repulsive Yukawa tail interactions, and focus on small densities. The relative increase of the temperature at the critical cluster concentration near the attractive surface (CCCS) shows a power-law dependence on the strength of the wall-particle attraction. At temperatures below the CCCS, the adsorbed layer consists of undeformed clusters if the wall-particle attraction is not too strong. Above the CCCS, or for strong attraction leading to flattening of the adsorbed aggregates, we obtain a monolayer that for strong or very strong attraction consists of flattened clusters or stripes respectively. The accumulated repulsion from the particles adsorbed at the wall leads to a repulsive barrier that slows down the adsorption process, and the accession time grows rapidly with the strength of the wall-particle attraction. Beyond the adsorbed layer of particles, a depletion region of a thickness comparable with the range of the repulsive tail of interactions occurs, and the density in this region decreases with increasing strength of the wall-particle attraction. At larger separations, the exponentially damped oscillations of density agree with theoretical predictions for self-assembling systems. Structural and thermal properties of the bulk are also determined. In particular, a new structural crossover associated with the maximum of the specific heat, and a double-peaked histogram of the cluster size distribution are observed.

Temperature-abnormal diffusion in tilted periodical potentials

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The phenomena of diffusion play a key role in a number of processes in physics, chemistry and biology. Our intuitive notion of the diffusion tells us that diffusion processes pick up speed with an increase in temperature. Meanwhile, this statement is unfair for the systems that are far from equilibrium. In this talk the systems with a different level of friction have been investigated. A set of original theoretical results on diffusion enhancement of underdamped Brownian particles in tilted space-periodic potential is presented [1–4]. It was established that the systems with a low friction level γ' show temperature abnormal diffusion (TAD) at which the diffusion coefficient D is increased with a decrease in temperature. This talk studies how the transition from the exponential relationship of TAD to the ordinary power temperature relationship occurs with an increase in γ'. It was shown that the energy barrier ε separating "running" and "localized" solutions is decreased with an increase in the friction coefficient At $\gamma' > 1.1$ the value of ε is close to zero.

It was established that the temperature "window" of TAD appears in the domain of the intermediate values of friction coefficient $0.1 < \gamma' < 1.1$. In a certain range of forces the diffusion coefficient is first increased with a drop in temperature and then it drops again. The diagrams of the existence of such domains were constructed.

The obtained data open the prospects for the creation of new technologies used for the control of diffusion processes.

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A metal film on a dielectric substrate within jellium model

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The thin metal films on dielectric or semiconductor substrates demonstrate properties that are interesting both from the point of view of fundamental science and from the perspectives of their technical applications in nanosized electronic devices.

One of the methods for a theoretical study of thin metal films is the use of model potentials, which are simple enough both to solve the stationary Schrödinger equation analytically and qualitatively correctly reflect the physical picture, namely, they do not allow electrons to leave a metal film [1].

The chemical potential and the work function of an aluminium metal film which is in the vacuum (1) and on a dielectric substrate (2) are obtained using the model of non-interacting electrons limited by an asymmetric rectangular potential well. For the first time, these two characteristics are calculated with correct taking into account the electroneutrality condition. As a result, the values of the chemical potential and the work function tend to their bulk values upon increasing the film thickness. The presence of a dielectric substrate leads to a small shift in the values of these characteristics [2].

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Combining pump/probe PES and electronic Raman scattering to test for the thermalization of hot electrons

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In a pump/probe experiment, the sample is hit with an intense electromagnetic pulse that excites electrons to a nonequilibrium state and then another pulse is applied after some time delay to probe the system. This allows one to study the relaxation processes of different excitations which are present in the system. Here, we propose a practical *in situ* method that can directly test for whether elecrons have thermalized. The underlying idea is that effective temperatures of all the bosonic and fermiomic excitations must be the same when the system is in thermal equilibrium. These effective temperatures can be directly extracted from the photoemission spectra (single-particle excitations, fermionic) and the electronic Raman scattering cross section (two-particle excitations, bosonic) and compared to each other on an ultrafast time scale.

To illustrate how this works, we solve for the time-resolved nonresonant electronic Raman scattering cross section in the B_{1g} symmetry channel and compare this to similar time-resolved photoemission. The calculations are exact for the spinless Falicov-Kimball model within nonequilibrium dynamical mean-field theory. We perform calculations for different Coulomb interactions which determine different phases of the model in equilibrium (strongly correlated metal or insulator).

Determination of free energies of point defects by molecular dynamic simulation: Case of nickel

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At equilibrium all materials are characterized by presence of vacancies. Although the equilibrium concentration of vacancies is in general small, extra concentrations may be gen- erated by various processes when the material is acted upon by external agents, such as quenching, irradiation, oxidation, corrosion, and stress. Condensation and configuration of vacancy clusters play an important role in the evolution of damage in a variety of materials. In nickel experimental studies have shown the influence of point defects on the oxidation process. The hypothesis put forth by these experimenters to explain this phenomenon rests on an increased diffusion of oxygen inside the alloy, this being driven by a strong interaction between oxygen and vacancies. These are the vacancies present initially in the alloy, but also the ones injected at the metal-oxide interface during the oxidation process. Experimental characterization of point defects is often hindered by the limited resolution of the techniques in use, and also by the simultaneous presence of several kinds of defects in the system. Numerical simulations allow to isolate a defect of some kind and study it in detail. Therefore, simultation studies offer a valuable complement to experiments. However, so far finite temperature results are confined to those obtained using the quasi-harmonic approxi- mation, whose validity is limited to low temperatures. In this work we perform free energy calculations to study the stability of a divacancy in nickel at relatively high temperatures. We use well-tempered metadynamics with an embedded atom potential for direct free energy estimations. The main result is that the divacancy, while stable at low temperature, will dissociate at high enough temperature. The low temperature result is in agreement with the results obtained using the quasi-harmonic approximation. However, it is to be expected that the two methods will differ at high temperature.

Van der Waals equation of state for hard-sphere system: A new twist to the old story

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For the system of hard-sphere particles the van der Waals equation of state is generalized to include the dependence of the excluded volume parameter on density. Analytical approximations are obtained for the parameter and shown to improve the accuracy of the equation. The results are tested against Monte Carlo simulations. Excluded volume is seen to drop by a factor of 2 over the density range where the system is still in the fluid state. Partial contributions of two- and three-sphere intersections to the excluded volume are analyzed. Implications of the obtained results for systems with attractive interactions and systems interacting via continuous potentials are discussed.

Thermodynamics of frustrated Heisenberg magnets on the kagome and pyrochlore lattices: Green's function approach and high-temperature expansion

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Heisenberg models on highly frustrated lattices are in the focus of many theoretical studies. While there are numerous studies of the ground state of the kagome and pyrochlore lattices, much less is known about the thermodynamic properties. We use the spin-rotation invariant Green's function method [1–5] as well as the high-temperature expansion up to order 13 [6] to study the temperature dependence of the magnetic structure factor $S_{\mathbf{Q}}$, the uniform susceptibility χ_0, the specific heat C_V, the correlation length ξ_Q and the correlation functions $\langle S_{\mathbf{0}} S_{\mathbf{R}} \rangle$ for $S \geq 1/2$ of the Heisenberg antiferromagnet on the kagome [4] and pyrochlore [5] lattices as well as the Heisenberg ferromagnet [3] on the pyrochlore lattice for arbitrary spin quantum number S.

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On solving the moment master equations of population dynamics for spatially inhomogeneous systems

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The problems of solving the master equations for population dynamics of spatially inhomogeneous birth-and-death systems with nonlocal dispersal and competition are considered. It is shown that the standard numerical methods working well at spatially homogeneous conditions are unsuitable when studying the spatial inhomogeneity beyond the mean field approximation. The account of this inhomogeneity is mandatory for the wavefront and spread dynamics, in ecological invasions, in vitro cell invasion assays, embryogenesis and wound healing, malignant tumor proliferation, etc [1]. Despite the previous achievements, very little remains known about spatial moment dynamics of inhomogeneous systems.

In order to remedy such a situation, we propose a novel approach to find the desired solutions using analytically solvable decompositions of the time evolution operator. This has allowed us to calculate the inhomogeneous pair correlation functions of birth-and-death populations within the Kirkwood superposition moment closure for the first time. Also, we revealed a number of new subtle effects, possible in real systems. Namely, for populations with short-range dispersal and mid-range competition, strong clustering of entities at small distances followed by their deep disaggregation at larger separations are observed in the wavefront of density propagation. For systems in which the competition range is much shorter than that of dispersal, the pair correlation functions exhibit a long-tail behavior. Remarkably, the latter effect takes place only due to the spatial inhomogeneity and thus was completely unknown before. Moreover, both effects get stronger in the direction of propagation. All these types of behavior are interpreted as a trade-off between the dispersal and competition in the coexistence of reproductive pair correlations and the inhomogeneity of the density of the system.

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Bose polaron in ideal Bose gas at finite temperature

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When the impurity atom interacts with the Bose environment it forms quasiparticle called Bose polaron. Important progress in investigation of single Bose polarons experimental possibility control by parameters of the Bose bath and directly observe by behavior of the impurity atom [M. G. Hu, Phys. Rev. Lett. **117**, 055301 (2016); N. B. Jorgensen, Phys. Rev. Lett. **117**, 055302 (2016)]. The approximate theoretical methods and Monte Carlo simulations give us a complete picture for the explanation of properties of Bose polarons at low temperatures.

The behavior of the Bose polaron at finite temperatures is interesting, but almost not studied, because of features arising in the region of critical point, where the Bose system undergoes superfluid transition. Particularly, in [N. E. Guenther, Phys. Rev. Lett. **120**, 050405 (2018)] two branches of spectrum of the attractive Bose polaron in the case strong of boson-impurity interaction were discovered. The infrared behavior of Green's function of Bose polaron weakly coupled to the dilute D-dimensional gas in close vicinity of the Bose–Einstein condensation transition temperature was studied in [V. Pastukhov, J. Phys. A: Math. Theor. **51** 195003 (2018)]. In the work [J. Levinsen, Phys. Rev. A. **96**, 063622 (2017)] the authors show, by means of the second order perturbation theory in terms of the boson-impurity coupling parameter applied to a mobile impurity immersed in Bose gas, that the self energy of the Bose polaron in the region of critical temperature is divergent. In order to explain the physical nature of the above mentioned features of the Bose polaron spectrum we considered a simplified model of an impurity immersed in the ideal gas of bosons at temperatures close to the Bose–Einstein condensation transition point. By using of the non-self-consistent t-matrix approach we found out that the binding energy and life-time of the impurity loaded in Bose gas remain finite even in the critical region.

Equilibrium properties of a two-component Fermi gas coexisting with Bose-Einstein condensate of its heteronuclear bound states

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We study the equilibrium properties of ultracold two-component Fermi gas coexisting with Bose–Einstein condensate of heteronuclear bound states formed from its fermionic atoms [1]. To this end, we propose a microscopic approach that involves the Bogoliubov model for a weakly interacting Bose gas [2] and approximate formulation of the second quantization method in the presence of bound states of particles elaborated earlier by the authors [3]. The basic thermodynamic characteristics of the system such as the ground-state energy, the single-particle excitation spectra, the densities of molecular condensate and unbound fermionic atoms are found. The applicability conditions of the elaborated approach are discussed. The obtained results are applied to study a mixture of ^{6}Li and ^{173}Yb atoms. The quantum degeneracy of this mixture was realized experimentally that provides a good basis for creation of ultracold molecules with their subsequent condensation [4].

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Statistical model of a flexible inextensible polymer chain: the effect of kinetic energy

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Because of the holonomic constraints, the kinetic energy contribution in the partition function of an inextensible polymer chain is difficult to find, and it has been systematically ignored. We present the first thermodynamic calculation incorporating the kinetic energy of an inextensible polymer chain with the bending energy [1]. To explore the effect of the translation-rotation degrees of freedom, we propose and solve statistical model of a fully flexible chain of $N + 1$ linked beads which, in the limit of smooth bending, is equivalent to the well-known worm-like chain model. The partition function with the kinetic and bending energies and correlations between orientations of any pair of links and velocities of any pair of beads are found. This solution is precise in the limits of small and large rigidity-to-temerature ratio b/T . The last exact solution is essential as even very "harmless" approximation results in loss of the important effects when the chain is very rigid. For very high b/T, the orientations of different links become fully correlated. Nevertheless, the chain does not go over into a hard rod even in the limit $b/T \to \infty$: while the velocity correlation length diverges, the correlations themselves remain weak and tend to the value $\propto T/(N + 1)$. The N dependence of the partition function is essentially determined by the kinetic energy contribution as predicted in [2]. We demonstrate that to obtain the correct energy and entropy in a constrained system, the T derivative of the partition function has to be applied before integration over the constraint-setting variable.

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Computational modeling of memory effects in turbulent flows

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Numerous examples suggest that the Navier–Stokes equations $\mathbf{div}\, v = 0$, $dv/dt = \triangle v - \mathbf{grad}\, p + f$, where d/dt stands for total time derivative, is unable to govern the phenomenon of turbulence. There is observed on experiment the development of a turbulence, whereas on a sheet of paper the corresponding initial-boundary value problem posses smooth (regular), unique and stable to a reasonable perturbations of data, solution. So that the turbulization of a flow might not be ascribed to any experimental errors whatsoever. On the other hand, the infinite chain of Reynolds equations with averaged velocity of a flow being expressed through double correlation functions of random pulsations, double correlation functions — through triple correlation functions and so on, is believed by many to be capable of describing turbulence. We propose the way of **exact** splitting of Reynolds equations and treat the turbulence of a fluid flow as a two phase hydrodynamical system. The title of the talk reads: "Computational modeling …" In fact, our research involves some ideas and methods of numerical analysis, rather than the usage of computer itself.

Novel phase transitions in chemically heterogeneous slits

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Capillary condensation, i.e. condensation of vapor below the saturation pressure of fluids confined in a capillary slit is a well understood phenomenon which serves as a paradigmatic model for finite-size shifted phase transitions. In this work, we generalize this model to the case, when the slit walls are chemically heterogeneous and are formed of two species of different wettability. Using microscopic density functional theory (DFT), we show that the resulting phase behavior becomes very complex even in the case when the two plates are completely symmetric. Rather than just simple capillary condensation, as in the homogeneous case, the model experiences several phase transitions, such that the full condensation of the fluid inside the slit is preceded by intermediate states characterized by a formation of bridges either *along* or *between* the walls. The stability of these states depending on the geometric parameters of the walls and the distance between the walls is discussed and compared with the analytic prediction based on a mesoscopic analysis.

Morphological and bridging transitions at nanopatterned walls

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Using microscopic density functional theory (DFT) we study adsorption of a Lennard-Jones-like fluid at planar but chemically heterogeneous walls. The wall is formed of periodically alternating stripes of two different materials, one of which is completely wet ("solvophilic") and the other completely dry ("solvophobic") which are both of molecular widths. We consider two experimentally accessible scenarios: i) when the total amount of the adsorbed fluid is fixed, the fluid may adopt various configurations that are separated by a sequence of weakly first-order morhpological transitions; ii) when the system is open and can freely exchange particles with the bulk, the system undergoes bridging transition corresponding to a connection of small liquid droplets adsorbed on the wettable stripes over the hydrophobic gaps. We construct corresponding phase diagrams, analyze the shape of the liquid droplets and discuss the relevance of the macroscopic Cassie law.

Fine-structure oscillations in catalytic carbon monoxide oxidation on platinum

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A mathematical model for reaction-diffusion processes of carbon monoxide (CO) oxidation on the platinum (Pt) catalyst surface is constructed and investigated. It takes into account:

- the peculiarities of the Langmuir-Hinshelwood mechanism for a chemical reaction;
- the two-dimensionality of the surface on which the catalytic oxidation reaction takes place;
- the finiteness of the rate of reaction product (CO_2) desorption from the Pt surface.

The spatial and temporal periodic chemical oscillations of CO, oxygen, CO_2 surface coverages and the fraction of the catalyst surface in the nonreconstructed structure (1×1) are revealed. The influences of structural changes and inhomogeneities of the catalyst surface on the oscillatory character of reaction are investigated. It is shown that inhomogeneities lead to a fine structure.

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Ising model with invisible states on scale-free networks

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We consider the Ising model with invisible states on scale-free networks [1]. Our goal is to investigate the interplay between the entropic and topological influence on a phase transition. The former is manifest through the number of invisible states r, while the latter is controlled by the network node-degree distribution decay exponent λ. We show that the phase diagram, in this case, is characterised by two marginal values $r_{c1}(\lambda)$ and $r_{c2}(\lambda)$, which separate regions with different critical behaviours. Below the $r_{c1}(\lambda)$ line the system undergoes only second order phase transition; above the $r_{c2}(\lambda)$ only a first order phase transition occurs; and in-between the lines both of these phase transitions occur at different temperatures. This behaviour differs from the one, observed on the lattice, where the Ising model with invisible states is only characterised with one marginal value $r_c \simeq 3.62$ separating the first and second order regimes [2].

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Two-species reactive lattice gases on random catalytic chains: Annealed versus quenched disorder

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Catalytically activated reactions involve particles that react only in the presence of another agent, which is called a catalyst. Such catalytic processes are widespread in the nature and different technological applications. To study the properties of equilibrium and out of equilibrium properties of such reactions is devoted a lot of attention. In particular, it is known that the thermodynamic properties of the monolayers of adsorbed molecules, formed in the course of catalytically-activated reactions, are very similar to the properties of the adsorbates modelled by athermal hard core lattice gases. Therefore we study a lattice-gas model of two species particles and focus on the equilibrium properties of a catalytically activated $A + B \to 0$ reaction. Particles A and B, involved in the reaction, being in thermal contact with their vapor phases acting as reservoirs and may adsorb onto substrate and desorb from it. This process taking place on a substrate with some non-uniform catalytic properties. We consider the simplest case of reactions on a one-dimensional chain with some structural elements of which have catalytic properties. We consider that some bonds of a chain are catalytic and other case that some sites are catalytic. For both cases these structural elements placed randomly with mean concentration p. We consider two types of disorder in placement of catalytic elements when disorder can be viewed as annealed, and other case with a quenched random distribution of the catalytic elements. For both models we obtain the thermodynamic functions, namely the disorder-averaged pressure, particles density and the compressibility and compare obtained results for both types of disorder.

Porous silicon partly filled with water molecules: crystal structure, energy bands and optical properties from first principles

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We present the *ab initio* study of band structure and optical properties of porous silicon partly filled with water molecules. Our research is aimed at elucidating the evolution of the main electron structure properties of Si going from ordinary bulk three-dimensional material to porous state with ordered pores of a nanosize level. We are also interested in water structuring properties in the small Si pores, on the one hand, and the water impact on the energy band structure and optical properties of such nanocomposite compound represented by porous Si with water molecules inside the pores, on the other hand.

We investigated several periodic space morphologies of porous Si filled with water molecules as a function of pore diameter ranging from 7.5 to 15 Å, containing 8 to 24 H_2O molecules and the supercell including totally 91 to 211 atoms, respectively. Energy bands, density of states, high-frequency dispersion of dielectric permittivity, refractive indices, extinction coefficients and absorption spectra were calculated. We established that the energy band gap of porous Si mostly increases with increasing pore diameter. An embedding of water molecules into the pores of Si has insignificant impact on the energy band gap of such nanocomposite. However, we revealed significant changes in refractive indices and extinction coefficients when pores were filled with water. In general, the filling the pores with water molecules results in reduction of the tetrahedral space anisotropy of electron structure inherent to nanoporous Si.

Generalization of the Van der Waals equation for anisotropic fluids in a disordered porous medium

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We present a generalization of the Van der Waals equation of state for anisotropic fluids in a disordered porous medium. The generalized equation consists of two terms. The first of them is based on the equation of state for hard spherocylinders in random porous media obtained from the scaled particle theory and improved by Carnahan–Starling and Parson–Lee corrections [1]. The second term is expressed in terms of the mean value of anisotropic attractive interactions. The proposed generalized van der Waals equation is used for investigation of the gas-liquid-nematic phase behaviour of a molecular anisotropic fluids depending on the anisotropy of molecular shapes, the anisotropy of attractive intermolecular interactions and the porosity of porous medium [2]. It is shown that for sufficiently long spherocylinders the liquid-gas transition is located completely within the nematic region and leads to nematic-nematic phase separation. For all the considered cases the decrease of porosity shifts the phase diagram to the region of lower densities and lower temperature. The proposed generalization of the van der Waals equation is applied for description of the phase behaviour of solutions of a relatively rigid polypeptide, poly(γ-benzyl-*L*-glutamate) (PBLG), in dimethylformamide in porous media. A quantitative description of the experimental isotropic-nematic phase behaviour of the PBLG solutions is achieved using two temperature-dependent parameters. Some possible modifications of the phase behaviour by porous media are predicted [3].

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Hydrogen bonding between simple hydrides

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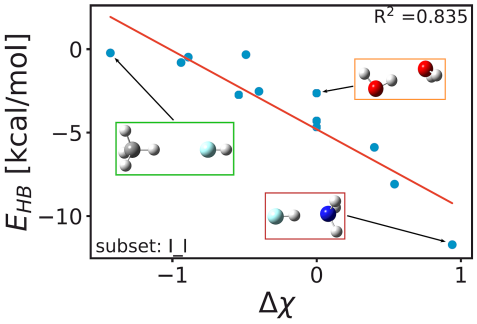
The hydrogen bond (HB) is one of the most important intermolecular interactions which gives a lot of substances its characteristic and also anomalous properties. Its effects can be observed from large biomolecules like nucleic acids, proteins, cellulose and other polymers, to simpler substances like liquid water where its effects are still quite complex. The common ground of all hydrogen bonded systems is the interaction between an electronegative element and a hydrogen atom which is bonded to another electronegative element. If we want to understand the HB on the macroscale we start with simpler systems and because it is not just a simple electrostatic interaction it should be evaluated on a quantum level (*ab initio* calculations).

In this work we calculated the HB strength of different dimeric hydrides (HCl, HF, HBr, H_2O, H_2S, H_2Se, NH_3, PH_3, AsH_3 and CH_4) using the MP2 method and Aug-cc-pVTZ basis set. The aim was to determine what influences the strength of strong as well as weak hydrogen bonds between those molecules. Various relationships were checked. A relation between the strength of the bond and the electronegativity of the participating atoms was found. We also observed a correlation between the strength of hydrogen bonds and the inter-atomic distances, along with the dependence on the charge transfer on the atom of the donor. We also provide characteristic geometries of evaluated dimers.



Arbitrary spin and statistics in the new relativistic wave equation, example spin $s = 3/2$

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Further approbation of the equation for the particles of arbitrary spin introduced recently in [1–3] is under consideration. The comparison with the known equations suggested by Bhabha, Bargmann–Wigner, Rarita–Schwinger (for spin $s = 3/2$) and other authors is discussed. The advantages of the new equations are considered briefly. The advantages follow from the fact that our equation does not contain the redundant components. The important partial example of spin $s = 3/2$ case is considered in details. The 8-component Dirac-like wave equation for the spin $s = (3/2, 3/2)$ particle-antiparticle doublet is suggested.

The Poincaré invariance and the way of introduction of interaction with external field is demonstrated.

The three level consideration (relativistic canonical quantum mechanics, canonical Foldy–Wouthuysen type field theory and manifestly covariant field theory) is presented.

The operator link between the relativistic canonical quantum mechanics and locally covariant field theory of arbitrary spin is found. Such link is given by the extended Foldy–Wouthuysen transformation between the $2(2s+1)$-component local field theory and the corresponding relativistic canonical quantum mechanics. On this basis the field equation is derived from the formalism of quantum mechanics. The hypothesis on the spin $s = 5/2$ particle is discussed.

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Summation theorem and its application to exact non-eqiulibrium full counting statistics of tunnel current in quantum-point contacts

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The central physical achievement of this study is exact analytical formula for time-dependent cumulant generating functional [1], which contains all information about quantum fluctuations in electron tunneling through arbitrary Luttinger liquid tunnel junction in the framework of Full Counting Statistics (FCS-) ideology [1–3]. In fact, this central result represents a first known exact analytical generalization of famous Levitov-Lesovik formula which was known previously only for the non-interacting electrons in tunnel junctions [3] — on the case of arbitrary electron-electron repulsion in one-dimensional Luttinger liquid quantum wires out of the equilibrium [1]. Exact analytical derivation [1] of this general formula makes use of the theorem about exact re-exponentiation of Keldysh-contour ordered T-exponent for Luttinger liquid tunnel junction, proven by the author (S-theorem) in Refs. [1,2]. The performed proof is the equivalent of exact microscopic proof of detailed balance theorem [3] for tunnel current of interacting electrons, which has never been performed in the literature before. Moreover, in a sufficiently broader context of nonequilibrium dynamics of interacting quantum fields in generic open quantum systems the exact and mathematically elegant re-exponentiation formula for fluctuating bosonic quantum field [1] — represents an important example of rigorous proof of very common and fundamental Jarzynski equality [4] in the real-time domain for quasi-one dimensional mesoscopic quantum systems out-of-the equilibrium [1]. As the important practical consequence of all mentioned general results the explicit picture of real-time quantum fluctuations decay in the process of the equilibration of tunnel current in arbitrary Luttinger liquid tunnel junction is performed.

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A review of Bogolyubov method of the reduced description of nonequilibrium states

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This year 110th Bogolyubov birthday is celebrated. In this talk a review of fundamental Bogolyubov ideas in nonequilibrium statistical mechanics is proposed with the following plan.

Natural evolution of a system and hierarchy of its nonequilibrium processes. Time scales separation.

Hilbert normal solutions and Bogolyubov idea of the functional hypothesis.

The Bogolyubov idea of the functional hypothesis as a basis of his method of the reduced description of nonequilibrium processes.

Chapman and Enskog ideas about natural evolution of nonequilibrium systems.

The Chapman–Enskog method of kinetic equation solution as some case of the Bogolyubov method of the reduced description.

The Grad method of kinetic equation solution and the Bogolyubov method of the reduced description.

The effective initial conditions to equations for parameters of the reduced description.

The reduced description of nonequilibrium processes in a system and invariant manifolds of this system.

Investigation by Bogolyubov of nonlinear system dynamics and the reduced description of nonequilibrium processes.

Bogolyubov idea of the functional hypothesis and Zubarev method in theory of nonequilibrium processes.

Investigation of nonequilibrium processes in a system with account for its kinetic modes.

Investigation of nonequilibrium processes in the vicinity of standard ones.

Correlations as parameters of the reduced description of nonequilibrium states.

Some of these themes can be omitted with account for time of the presentation.

Microscopic environment of the D205 dye in $BmimBF_4$ in ground and excited states

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The Dye-Sensitized Solar Cell (DSSC) is one of the cheap and easy alternatives for sustainable energy sources. It is based on the applying of room temperature ionic liquid both pure and mixed with molecular solvents as electrolytes and the indoline dyes that serve as antenna to harvest the photons of the incident light. It was shown that the dye D205 (Fig. 1) can be used in DSSC caused by high molar light absorption coefficient, electrochemical, photochemical and thermal stability for a long time, ability to absorb photons in all visible range, good solubility in molecular solvents and the presence of anchor -COOH group, binding to substrate.

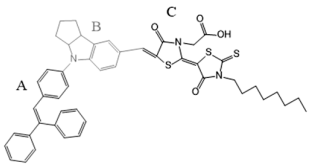

Figure 1: Dye D205: A-donor, B-bridge, C-acceptor

The efficiency of a DSSC depends on the properties of the excited state of the dye used, as well as its ability to electron transfer. All these characteristics are determined primarily by microsolvation of a dye in an electrolyte environment. Here we present the results of the investigation of D205 dye local solvation in ionic liquid $BmimBF_4$. To study the processes occurring at the microscopic level molecular dynamic (MD) simulations were performed by using GROMACS suit. A local solvation of the D205 molecule were analyzed in terms of radial, spatial and combined distribution functions using TRAVIS package. A special attention was paid to a comparison of ground and excited state of D205.

Low-frequency dynamics of one-dimensional systems with hydrogen bonds

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The frequency dependence of the dynamical susceptibility of the dipole-dipole type of the one-dimensional systems with hydrogen bonds is calculated using the Green's function formalism. The consideration is based on the hard-core boson model. We take into account short-range interactions between particles, and their transport along hydrogen bonds with the two minima local anharmonic potential as well as their inter-bond transfer. Calculations are performed for finite one-dimensional cluster with periodic boundary conditions using exact diagonalization technique. The vibrational spectra are studied depending on the particles (protons) tunneling frequency on the bond; the influence of transfer of particles between the bonds on these spectra is also investigated. The density of vibrational states is found, its frequency dependence is analyzed. In our 1d case we see, however, the absence of behaviour of the soft mode type. Instead of that, the new branch appears; it frequency is determined by energy of repulsion of protons.

Recent developments in the theory of electrodynamic homogenization of random particulate systems

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We present results [1–3], derived within the compact group approach (CGA) and effectively incorporating many-particle polarization and correlation effects, for the effective quasistatic dielectric constant/electrical conductivity of model dispersions of hard-core–penetrable-shell particles embedded in a continuous matrix. Both the cores and shells are characterized by radially symmetrical distributions of their electric parameters. The local properties of overlapping constituents are governed by the distance from a given point to the nearest particle.

Let x be an electric parameter of a system $\mathcal{D}$ and x_{eff} its effective value. The key points behind [1–3] are as follows:

(1) $\mathcal{D}$ is electrically equivalent to an auxiliary system $\mathcal{S}$ formed by embedding $\mathcal{D}$'s constituents into a uniform host with $x = x_{\text{f}}$. $\mathcal{S}$ is a set of macroscopic regions (compact groups) large enough to have the properties of the entire $\mathcal{S}$, but point-like relative to the probing field;

(2) x_{eff} is found as the proportionality coefficient in the relevant constitutive relation between the averaged induction/current and field. These averages are expressed through the statistical moments $\langle (x - x_{\text{f}})^n \rangle$;

(3) Combining the CGA with the Hashin-Shtrikman variational theorem or the boundary conditions for electric fields, x_{f} is proven to equal x_{eff}. This result makes the homogenization procedure internally closed;

(4) Finally, x_{eff}, as a functional of $\mathcal{D}$'s constituents' conductivities and volume concentrations, is shown to obey an integral relation, rigorous in the quasistatic limit.

We demonstrate the validity of our results by: (a) contrasting them with analytical and numerical results for dispersions of graded dielectric spheres with power-law permittivity profiles; (b) mapping them onto extensive random resistor network simulation data for composite polymer electrolytes; and (c) applying them to real composite electrolytes.

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Relation of entanglement of continuous variable graph states with graph properties

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Recently, continuous variable graph states attain considerable attention as a method of implementing a quantum computer. Unlike traditional quantum computation, which is based on discrete quantum variables and qubits, the continuous variable quantum computation is based on qumodes, quantum systems with an infinite-dimensional Hilbert space spanned by a continuum of orthogonal states.

In this report we are interested in the relation of quantum properties of continuous variable graph states with the properties of the underlying graph. To this end, we consider the graph states defined as

$$\psi(\mathbf{x}) = \psi(x_1, x_2, ..., x_N) = \sqrt{\frac{\alpha^N}{\pi^N}} \exp\left(-\sum_j \frac{\alpha}{2} x_j^2 + i \sum_{j \neq k} \frac{a_{jk}}{2} x_j x_k \right),$$

here α is constant, a_{ij} are elements of a constant symmetric matrix $\hat{a}$, indices $j, k = (1, ..., N)$. The state can be obtained as a result of action of the unitary operator $\hat{U}_{jk} = \exp(i a_{jk} x_j x_k)$ on the ground state of a system of N noninteracting harmonic oscillators. Each oscillator being represented by graph vertex, the last term in the exponent can be understood as a sum over graph edges. Subsequently, matrix $\hat{a}$ is the adjacency matrix of the graph.

We analyse the geometric measure of entanglement in the graph state and find that the entanglement of a harmonic oscillator with other ones is defined by the value of its vertex degree. We also study correlation of the Fubini–Study distance between the graph states with Hamming and Hilbert–Schmidt distances between the corresponding graphs.

Generalized diffusion equation with fractional derivatives. Zubarev's NSO method

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In Refs. [1–3], by using the Zubarev nonequilibrium statistical operator method [4] and the maximum entropy principle for the Renyi entropy, we consider a way of obtaining generalized (non-Markovian) diffusion equation with fractional derivatives. We found a solution of the Liouville equation with fractional derivatives [5] at a selected set of observed variables.

By modeling of memory function, a generalized diffusion equation of the Cattaneo–Maxwell type with fractional derivatives is obtained taking into account space-time non-locality. Dispersion relations for the diffusion equation of the Cattaneo–Maxwell type are found. A frequency spectrum, phase and group velocities of particles are calculated.

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On applicability of rotational band approximation

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Rotational band approximation (RBA) is valid for quantum antiferromagnetic Heisenberg model on finite bipartite lattices. It assumes that for lower energy levels $E_{min}(S) \approx cS(S+1)$. It's known that increasing number of lattice unit cells or introducing geometric frustration deteriorate this approximation, but it's not well understood how critical number of elementary cells or frustration strength depends on lattice structure.

Usage of eigendecomposition of exchange parameter matrix J allows us to write Heisenberg Hamiltonian in the following form

$$H = \sum_{\langle i,j \rangle} J_{ij} \mathbf{S}_i \mathbf{S}_j = \sum_{l=1}^{n} \lambda_l \sum_{\langle i,j \rangle} v_{li} v_{lj} \mathbf{S}_i \mathbf{S}_j,$$

where λ_l and $\mathbf{v}_l$ are eigenvalue and corresponding eigenvector of J.

We show that for d-regular bipartite expander graphs (namely bipartite double covers of strongly regular graphs) of any size RBA is valid at least for ground state energy E_0 in second order of perturbation theory in spectral parameter $\delta = \lambda_2/d$, where λ_1 is second largest eigenvalue of J.

For this type of lattices energy of ground and lower excited states of antiferromagnetic Heisenberg model with $S = const$ is accurately predicted by spin wave theory. We use the fact that spin wave energy and wavefunctions can be expressed as functions of $\lambda_l, \mathbf{v}_l$ and that eigenvectors $\mathbf{v}_l$ have definite lattice symmetry to perturbatively study influence of uniform frustration $J \to J + \alpha(J - dI)$ and approximate critical value of frustration parameter α_c that corresponds to quantum phase transition.

Effect of hydrostatic pressure and longitudinal electric field on dielectric properties of CDP ferroelectric

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The phase transition in the CsH_2PO_4 (CDP) crystal is caused by proton ordering on the hydrogen bonds. To study its dielectric properties we use the proton ordering model, which takes into account piezoelectric coupling of the proton subsystem with lattice strains ε_1, ε_2, ε_3 and ε_5. Within the two-particle cluster approximation we have calculated the dielectric characteristics of CDP under hydrostatic pressure and longitudinal electric field E_y.

Application of the hydrostatic pressure in the absence of the field leads to decreasing of the phase transition temperature T_c from the paraelectric to the ferroelectric phase. At the pressures higher than some critical one p_k there appears the phase transition from the paraelectric to the antiferroelectric phase at the temperature T_N, which also decreases with pressure. A satisfactory quantitative description of the experimental data is obtained.

The electric field E_y, which is applied additionally to the hydrostatic pressure, smears the ferroelectric phase transition, decreases the temperature T_N, increases the critical pressure p_k and longitudinal dielectric permittivity ε_{yy} in the antiferroelectric phase.

Dipole ordering and strain effects in the deformable Blume–Emery–Griffiths model

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Ferroelectrics belonging to the $Sn_2P_2S_6$ family (with the possible partial substitutions Sn → Pb and S → Se) are known for their sensibility to a hydrostatic pressure. The *ab initio* calculations showed that ionic groups P_2S_6 exist in three configurations (determined by their shape and distribution of electronic charge), which in the paraelectric phase are described by a symmetrical three-well potential in the configurational space. In the absence of external influence, the $Sn_2P_2S_6$ crystal exhibits the second order phase transition to the ferroelectric phase due to a dipole ordering of these structure elements. At the increase of pressure the temperature of the second order phase transition decreases, a tricritical point is achieved, and, finally, the ferroelectric state is suppressed.

For such a crystal we proposed a modified version of the BEG model taking into account the microscopic mechanism of the external pressure influence on thermodynamics and phase transitions in lattices with a three-well local lattice potential. We assume that the influence of pressure is not a direct one but it is mediated by the crystal lattice strain. Namely, the crystal deformation leads to the change of internal field and displacements of atoms surrounding the structure elements (ionic groups); configurations of the latter are determined by the mentioned above local potential. Our modification of the BEG model supplementarily considers the shift of local energy levels (due to restructuring of local anharmonic potentials) under the influence of deformation caused by a uniform pressure or tension. Such an approach allows to describe the deformational effects accompanying the phase transitions to the state with a dipole ordering (the ferroelectric phase).

Based on this model, the pressure dependences of the $u = \Delta V/V$ volume deformation are calculated for the $Sn_2P_2S_6$ crystal. The presence of anomalies of $u(p)$ function in the regions of ferroelectric phase transitions of the first and second order as well as the tricritical point is established; the behaviour of the volume compressibility is investigated. Metastability phenomena related to a possible hysteresis are also analysed. Obtained results are compared to the experimental data.

Effect of the bond distortion in the Ising-Heisenberg model on the Shastry-Sutherland lattice

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We consider a hybrid version of the distorted Shastry–Sutherland model with the Heisenberg intradimer and Ising interdimer couplings. We focus on the case where the bond distortions of the orthogonal dimers may lead to the different values of the intradimer couplings depending on the bond orientation. Using the unitary transformation [1] the model can be diagonalized and its ground state is found rigorously. We show that in zero magnetic field the bond distortion gives rise to the modulated antiferromagnetic phase previously observed also in the orthogonal-dimer chain, a one-dimensional counterpart of the Shastry–Sutherland model. The effect of the external magnetic field is also studied for the different ratio of the bond distortion. The ground-state phase diagram gains the 1/4-plateau phase in addition to the 1/3- and 1/2- plateaux obtained for the symmetric model [1]. We also show how the distortion suppress the stripe 1/3-plateau phase in favor of the 1/4- and 1/2-plateau phases.

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Thermodynamic and structural properties of systems with SALR interaction on two- and three-dimensional lattices

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Systems with competing interactions are appropriate for modelling biological objects (colloids, ensembles of protein molecules, etc.). The lattice system with attraction between nearest neighbors and repulsion between next-next-nearest neighbors on a square (sq) and simple cubic (sc) lattices is studied.

The competing interactions lead to the order-disorder phase transitions. The geometric order parameter for localizing the phase transition points is introduced for both systems. The critical values 0.655 and 0.186 of the interaction parameter J/k_BT_c for sq and sc lattices respectively were estimated. The phase diagrams of the systems were constructed. The chemical potential sharply changes in the phase transition region, while the thermodynamic factor indicates strong suppressing of fluctuations that is inherent for ordered states of the systems. The complicated behaviour of the correlation functions that reflect structural peculiarities of the system demonstrates an important contribution of competing interactions.

The simple quasi-chemical approximation is proposed for the system under consideration. The concentration versus chemical potential, the thermodynamic factor (the derivative of the concentration logarithm over the chemical potential), and the correlation functions are determined both within the framework of the developed approximate approach and as a result of the Monte Carlo simulation of the lattice system. The proposed analytical approach allows one to correctly describe the qualitative features of the structural properties of systems with competing interactions and can be used to quantify the thermodynamic characteristics of these systems.

The project has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Sklodowska-Curie grant agreement No 73427 and the Ministry of Education of Belarus. Discussions with Prof. A. Ciach are gratefully acknowledged.

Monte Carlo simulation of a 3D solid electrolyte on a simple cubic lattice: concentration and electric field distribution at and without an external field

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Solid electrolytes are widely used in rechargeable batteries, fuel cells, supercapacitors, to name a few. Accounting for long range Coulomb interactions is one of the challenges in their theoretical investigations. Additional difficulties appear due to their ceramic structure and presence of intergrain boundaries.

A three-dimensional (3D) model of a solid electrolyte is considered. It consists of a one-component electrolyte on a 3D simple cubic lattice with neutralizing static background. In addition to Coulomb interactions a short-range van der Waals interactions are taken into account. The ions perform thermally activated hops to vacant nearest neighbor lattice sites. The structural peculiarities of the system are reflected by an energetic landscape. The intergrain and near electrode regions are modelled by variations of site and intersite energies.

Monte Carlo simulations were performed for calculating the charge and concentration distribution at various thermodynamic conditions. The Ewald summation was used for accounting for the Coulomb interactions. The electric current and conductivity were estimated at open circuit conditions by the number of ions passed through the system.

The simulation results has allowed investigating the structure of electric double layers in intergrain and near electrode areas. They are compared with the results of more simple quasi-one-dimensional models [1,2].

The project has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Sklodowska-Curie grant agreement No 73427.

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Combined effect of 1.5- and double scatterings on the Rayleigh line width near the vapor-liquid critical point

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It is widely believed [1] that the spectrum of molecular light scattering near the vapor-liquid critical point (CP) is formed mainly by single and true multiple (successive reemissions by distant density fluctuations satisfying the wave-zone condition) scattering effects. In contrast, we argue [2–4] that these mechanisms must be complemented by the 1.5-scattering, formed by triplets of density fluctuations spaced by distances $r \ll r_c < \lambda$ (λ and r_c being the wavelength and the correlation radius in the fluid, respectively). This mechanism is of the most significance along noncritical isochores in the pre-asymptotic vicinity of the CP. The presence of 1.5-scattering in the overall scattering pattern was demonstrated in [3,4] by processing experimental data [5] on the depolarization factor for xenon and those [6] on the Landau-Plazcek ratio near the λ-line.

The results [3] also reveal an asymptotic nature of the iterative series for the overall scattering intensity: (1) the magnitudes of the 1.5 and double scattering intensities can become comparable with that of the single scattering intensity; (2) the first two intensities can have opposite signs, tending to compensate for each other.

In this report, results [3,4] are used to evaluate the spectral intensity distribution for the 1.5-scattering; reproduce that for the double scattering; and scrutinize the combined effect of both mechanisms on the overall spectrum. In particular, this effect can manifest itself in the form of a stronger narrowing (temperature dependence) of the Rayleigh line, compared to that in the single scattering spectrum, as the CP is approached. The corresponding critical exponent and multiplicative renormalization coefficient are estimated and compared with experiment.

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Molecular dynamics simulation of 1-1'-spirobipyrrolidinium tetrafluoroborate acetonitrile solutions

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Electric double-layer capacitors (EDLC) are perspective electrochemical storage of electronic energy due to high power density, short time of charge/discharge and long lifetime. It was established that acetonitrile (AN) solution of 1-1'-spiropyrrolidinium tetrafluoroborate ($SBPBF_4$) is a perspective electrolyte for the EDCLs due to higher conductivity as compared with analogs [1].

Here we present the results of the thorough investigation of microscopic structure of ionic subsystem and transport properties of the highly concentrated solutions of $SBPBF_4$ in AN by using atomistic molecular dynamics simulation (MD) and quantum theory of atoms in molecules (QTAIM) [2]. The cation force field model were generated by ATB [3] builder and then improved to represent conformational diversity. The anion's force field model is author's modification of well-known Wu [4] tetrafluoroborate with better reproduction of anion's spectral properties. All necessary quantum calculation we carried out on M062X/6-311++G(d,p) level theory. All MD simulations were carried out in NPT ensemble with temperature equal to 298.15 K and 1 atm pressure by using GROMACS package [5].

The results of MD simulation provide a deep insight into the concentration dependence of the transport properties of concentrated solutions of $SBPBF_4$ in AN. Using QTAIM analysis the hydrogen bonds between cation's hydrogens and anion's fluorines were proclaimed as the main interaction in ionic associates.

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Application of statistical physics methods to stochastic financial models

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As it is known the dynamics of financial assets, derivatives, and other indicators is described by stochastic equations. The Viner process (Brownian motion) plays the main role in financial stochastic analysis. As a rule the stochastic processes being considered are Markov processes. Hence it is sufficiently to know the conditional probability density to be able to describe characteristics of stochastic processes. Conditional probability density satisfies the Fokker–Planck equation. In dynamics of physical processes the stochastic equations are also known as Langevin's equations. For imaginary time the Fokker–Planck equation is equivalent to a Schrodinger equation of a quantum-mechanical system. The method of Feynman (continuum) integrals is effectively used to solve Fokker–Planck equations and Schrodinger equations (system evolution). In method of continuum integration boundary conditions are taken into account quite effectively for propagator of a quantum system as well as for conditional probability density. Particularly, Dirichlet and Neumann boundary conditions can be taken into account by introducing additional 'potentials' which are expressed through delta function $\delta(x)$ and its derivative $\delta'(x)$ respectively. In this article the mentioned approaches are used to model a structure of interest rate and bonds yield. Mentioned problems were solved for a number of stochastic models, Merton model, Vasicek modes and others. In Merton model the dynamics of interest rate is described by a Brownian motion with drift. Vasicek model of interest rate is an analogue to a known Ornstein–Uhlenbeck model of statistic physics. However received solutions have significant drawbacks as they allow negative values of interest rate. As the result in Merton model the interest rate increases in time unlimitedly. In given approach the Dirichlet boundary condition for $r = 0$ is taken into account by introducing a potential $\delta(r)$ in continuum integral for conditional probability density, which limits the value of interest rate by domain $r > 0$. Continuum integral for conditional probability density is obtained by means of substitution in integral based on Wiener measure. As a result a time structure of interest rate was determined and a correct behavior of Merton model was obtained.

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5-та наукова конференція
“Статистична фізика: сучасні напрямки та застосування”

Львів, 3–6 липня 2019 р.

Програма і тези доповідей

Комп’ютерне макетування: Андрій Швайка

Графічне оформлення: Олеся Мриглод, Данило Добушовський

Укладання: Олег Величко

Формат 84×108/32. Ум. друк. арк. 11,6.
Друк офсетний. Тираж 250 прим.

Timetable of the 5th Conference "Statistical Physics: Modern Trends & Applications"

July 3, Wednesday		July 4, Thursday		July 5, Friday		July 6, Saturday	
$09^{00} - 13^{00}$	**Registration of the StatPhys-2019 participants**	$09^{00} - 09^{40}$ $09^{40} - 10^{05}$ $10^{05} - 10^{30}$ $10^{30} - 10^{45}$ $10^{45} - 11^{00}$	**Chaired by C. Pierleoni** Giovanni Ciccotti Sara Bonella Ruslan Davidchack Hong XU Alexander Vidybida	$09^{00} - 09^{40}$ $09^{40} - 10^{05}$ $10^{05} - 10^{30}$ $10^{30} - 10^{45}$ $10^{45} - 11^{00}$	**Chaired by J. Richter** Sergej Flach Masud Haque Oleksiy Kolezhuk Volodymyr Pastukhov Andrii Sotnikov	$09^{00} - 09^{40}$ $09^{40} - 09^{55}$ $09^{55} - 10^{25}$ $10^{25} - 10^{45}$ $10^{45} - 11^{00}$	**Chaired by N. Jakse** Giancarlo Ruocco Alexander Krivchikov Leonid Ponomarenko Jurij Kozicki Vadim Ohanyan
		$11^{00} - 11^{30}$	**Coffee break**	$11^{00} - 11^{30}$	**Coffee break**	$11^{00} - 11^{30}$	**Coffee break**
		$11^{30} - 12^{10}$ $12^{10} - 12^{50}$ $12^{50} - 13^{15}$ $13^{15} - 13^{30}$	**Chaired by J. Kozicki** Ralph Kenna Jozef Sznajd Miguel A.F. Sanjuán Maxym Dudka	$11^{30} - 12^{10}$ $12^{10} - 12^{35}$ $12^{35} - 13^{00}$ $13^{00} - 13^{15}$ $13^{15} - 13^{30}$	**Chaired by G. Ciccotti** Ari Seitsonen Oleg Kalugin Noel Jakse Jean-François Wax Miha Lukšič	$11^{30} - 12^{10}$ $12^{10} - 12^{50}$ $12^{50} - 13^{15}$ $13^{15} - 13^{30}$	**Chaired by Yu. Kalyuzhny** Marina Saphiannikova Dung di Caprio Stefan Sokolowski Svyatoslav Kondrat
		$13^{30} - 15^{00}$	**Lunch**	$13^{30} - 15^{00}$	**Lunch**	$13^{30} - 15^{00}$	**Lunch**
$13^{00} - 13^{10}$	**Opening ceremony**	$15^{00} - 15^{40}$ $15^{40} - 16^{05}$ $16^{05} - 16^{20}$	**Chaired by A. Ciach** Gerhard Kahl Wojciech Gozdz Vyacheslav Vikhrenko	$15^{00} - 15^{40}$ $15^{40} - 16^{05}$ $16^{05} - 16^{20}$	**Chaired by G. Ruocco** Carlo Pierleoni Anatoly Belonoshko Oleksii Rebenko	$15^{00} - 15^{40}$ $15^{40} - 16^{05}$ $16^{05} - 16^{20}$ $16^{20} - 16^{45}$	**Chaired by R. Kenna** Alain Dutech Maciej Koch-Janusz Maksym Druchok Krzysztof Kułakowski
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