Dedicated to the 100th Anniversary
of Professor Ihor Yukhnovskii

StatPhys 2025

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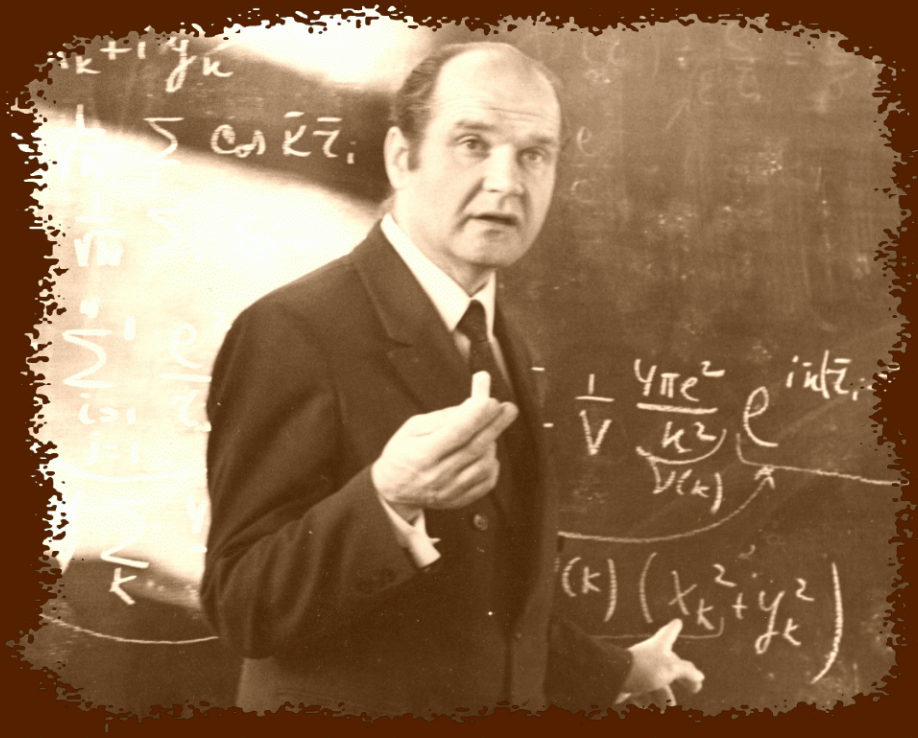

The 6th Conference

Statistical Physics: Theory and Computer Simulations

27–29 August 2025, Lviv, Ukraine

Programme and Abstracts

The 6th Conference

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Dedicated to the 100th Anniversary of Professor Ihor Yukhnovskii

PROGRAMME AND ABSTRACTS

Lviv – 2025

The 6-th International Conference "Statistical Physics: Theory and Computer Simulations" will take place in Lviv, Ukraine on August 27–29, 2025 and will be jointly organized by the Yukhnovskii Institute for Condensed Matter Physics of the National Academy of Sciences of Ukraine, Ivan Franko National University of Lviv, and Lviv Polytechnic National University. The Conference will be held in the Main building of Lviv Polytechnic National University (12 Stepan Bandera Str., Lviv).

This Conference continues a tradition of regular international meetings in statistical physics in Ukraine, established in the 1970-ies and renewed by "Statistical Physics" (Lviv, 2005; Kharkiv, 2006; Lviv, 2009, Lviv, 2012 and Lviv, 2019). The 2025 edition holds special significance as it is dedicated to the 100th anniversary of Professor Ihor Yukhnovskii, an eminent Ukrainian physicist, politician, and the founder of the Yukhnovskii Institute for Condensed Matter Physics.

The Conference will consist of invited lectures (40 min), key note and contributed talks (30–20 min) and poster presentations. Official language of the Conference is English.

Main topics

- Complex Systems
- Computer Simulations
- Quantum Matter and Quantum Technologies
- Soft Matter

Contacts

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Organizers

Yukhnovskii Institute for Condensed Matter Physics
Ivan Franko National University of Lviv
Lviv Polytechnic National University

Supported by

The National Academy of Sciences of Ukraine
The Ministry of Education and Science of Ukraine
Lviv City Council

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O. Velychko

Conference History

This Conference continues a tradition of the regular workshops in the statistical physics in Ukraine, established in the 1970s 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 the 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).
- **The 5th Conference "Statistical Physics: Modern Trends and Applications"**, July 3–6, 2019, Lviv, Ukraine (dedicated to the 110th birthday of the famous theoretical physicist and mathematician Mykola Bogolyubov, founder of the Bogolyubov Institute for Theoretical Physics (Kyiv)).

The 6th Conference

"Statistical Physics: Theory and Computer Simulations"

Programme

27–29 August 2025, Lviv, Ukraine

Wednesday, August 27, 2025
Lviv Polytechnic National University, Main building,
Matejko hall (Assembly hall)

08:00 – 09:00 Registration of the "StatPhys-2025" participants

09:00 – 09:40 OPENING CEREMONY

Chaired by T. Bryk *(Lviv, Ukraine)*

09:40 – 10:20 G. Ciccotti *(Rome, Italy)*
Hydrodynamic simulations and hydrodynamic limit of the scattering function via time-dependent non-equilibrium molecular dynamics

10:20 – 11:00 A.A. Kordyuk *(Kyiv, Ukraine)*
Searching for new quantum materials: Theory-guided approach with synchrotron ARPES

11:00 – 11:20 CONFERENCE PHOTO

11:20 – 11:40 Coffee Break (room 231)

Chaired by A. Zagorodny *(Kyiv, Ukraine)*

11:40 – 12:10 W. Ebeling *(Berlin, Germany; online)*
Statistical theory of charged particle systems including triple bound states — and the collaboration Lviv–Rostock

12:10 – 12:40 M. Holovko *(Lviv, Ukraine)*
On the contribution of I. Yukhnovskii to the development of statistical theory of electrolyte solutions

12:40 – 13:10 J. Kozicki *(Lublin, Poland)*
Fifty years of Yukhnovskii's critical point theory

13:10 – 13:40 O. Pizio *(Mexico, Mexico)*
Modeling of adsorption of water on solid surfaces chemically modified by grafting of chain molecules

13:40 – 15:00 Lunch

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

15:00 – 15:40 M.P. Allen *(Coventry, United Kingdom; online)*
Molecular simulation of liquid crystals in periodic boundary conditions

15:40 – 16:20 M. Bonitz *(Kiel, Germany; online)*
Nonequilibrium Green functions simulations of femtosecond dynamics of quantum materials

16:20 – 17:00 A.B. Belonoshko *(Nanjing, China)*
Impact of magnetism account on computation of iron phase diagram

17:00 – 17:20 Coffee Break (room 231)

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

17:20 – 18:00 U.C. Täuber *(Blacksburg, USA; online)*
Stochastic population dynamics of competing species in driven and/or spatially inhomogeneous systems

18:00 – 18:40 J.K. Freericks *(Washington, USA; online)*
Using quantum computers to prepare ground states of the Hubbard model and in quantum chemistry

19:00 – 21:00 GET-TOGETHER PARTY

Thursday, August 28, 2025
Lviv Polytechnic National University, Main building,
Matejko hall (Assembly hall)

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

09:20 – 10:00 J.J. Ruiz-Lorenzo *(Badajoz, Spain; online)*
Multifractals in statistical mechanics

10:00 – 10:40 V. Dotsenko *(Paris, France)*
On the scaling properties of (2+1) directed polymers

10:40 – 11:20 A. Ciach *(Warsaw, Poland; online)*
Mesoscopic theory for concentrated ionic systems

11:20 – 11:40 Coffee break (room 231)

Chaired by A. Sotnikov *(Kharkiv, Ukraine)*

11:40 – 12:20 J.-U. Sommer *(Dresden, Germany; online)*
Biomolecular condensates and the physics of polymers in mixed solvents

12:20 – 13:00 A.P. Seitsonen *(Paris, France)*
Collective dynamics in liquid water from computer simulations using molecular dynamics

13:00 – 13:40 S.G. Sharapov *(Kyiv, Ukraine)*
Sagnac effect in graphene

13:40 – 15:00 Lunch

Lviv Polytechnic National University, Main building,
Matejko hall (Assembly hall)

SOFT MATTER

Chaired by M. Holovko *(Lviv, Ukraine)*

15:00 – 15:30 A. Baumketner *(Lviv, Ukraine)*
Modeling aggregation of amyloidogenic proteins by computer simulations

15:30 – 16:00 T. Patsahan *(Lviv, Ukraine)*
Chelation of divalent heavy metal ions in aqueous environment

16:00 – 16:20 B. Lev, V. Yakovliev *(Kyiv, Ukraine)*
Linking diffusion to cyanide biodegradation kinetics

16:20 – 16:40 M.Ya. Sushko *(Odesa, Ukraine)*
A model for the effective dielectric response of granular mixtures

16:40 – 17:00 Coffee break (room 231)

Chaired by O. Pizio *(Mexico, Mexico)*

17:00 – 17:20 Y. Kalyuzhnyi *(Ljubljana, Slovenia; online)*
Polymerizing hard spheres with double shielded attractive shell

17:20 – 17:40 O. Patsahan *(Lviv, Ukraine)*
Spontaneous pattern formation in mixtures with competing interactions

17:40 – 18:00 A. Trokhymchuk *(Ljubljana, Slovenia)*
A novel approach to the reference equation of state for real fluids

Lviv Polytechnic National University, Main building,
Ju. Zachariewicz hall (room 214)

COMPLEX SYSTEMS

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

15:00 – 15:30 A. Rovenchak *(Lviv, Ukraine)*
Topological resilience and thermodynamic signatures in virus–host interaction networks

15:30 – 16:00 M. Dudka *(Lviv, Ukraine)*
Criticality of structurally-disordered spin systems with weak long-range interactions

16:00 – 16:20 T. Holovatch *(Lviv, Ukraine)*
Breakdown of hydrodynamics in a one-dimensional cold gas

16:20 – 16:40 I.T. Ersoy; online *(Potsdam, Germany)*
Geometry of learning: L2 phase transitions in deep and shallow neural networks

16:40 – 17:00 Coffee break (room 231)

Chaired by V. Dotsenko *(Paris, France)*

17:00 – 17:20 O. Vidybida *(Kyiv, Ukraine)*
Olfactory receptor neuron stimulated with Markov process

17:20 – 17:40 O. Borysenko *(Kharkiv, Ukraine)*
Application of Langevin dynamics for stochastic optimization in machine learning

17:40 – 18:00 A.V. Hlushchenko *(Kharkiv, Ukraine)*
Stochastic dynamics of magnetic textures on the racetrack memory

Lviv Polytechnic National University, Main building,
lobby of the second floor

18:00 – 19:00 POSTER SESSION

19:30 – 22:00 CONFERENCE DINNER

Friday, August 29, 2025
Lviv Polytechnic National University, Main building,
Matejko hall (Assembly hall)

COMPUTER SIMULATIONS

Chaired by A.P. Seitsonen *(Paris, France)*

09:20 – 09:50 J. Paturej *(Chorzów, Poland)*
Topology-driven self-assembly in cyclic polymers

9:50 – 10:20 S. Perepelytsya *(Kyiv, Ukraine)*
Electrical conductivity of DNA-counterion systems: theory and computer simulations

10:20 – 10:50 O. Kalugin *(Kharkiv, Ukraine)*
Microscopic structure, solvation and transport properties of LiFSI and LiFTFSI in EMC and NDF solutions: MD simulation

10:50 – 11:20 M. Druchok *(Lviv, Ukraine)*
Electric field effects on the quasiphase transition of confined water in single-wall carbon nanotubes

11:20 – 11:40 Coffee break (room 231)

Chaired by S. Perepelytsya *(Kyiv, Ukraine)*

11:40 – 12:10 V. Blavatska *(Lviv, Ukraine)*
Coagulation-flocculation process on a lattice: Monte Carlo simulations

12:10 – 12:40 J. Ilnytskyi *(Lviv, Ukraine)*
Computer simulations of adsorption of low density lipoproteins on a photosensitive polymer brush

12:40 – 13:00 A.I. Krivchikov *(Kharkiv, Ukraine)*
Absence of a boson peak in low-temperature heat capacity of some layered materials

13:00 – 13:20 Ya. Shchur *(Lviv, Ukraine)*
Lattice dynamics of $Bi_{12}SiO_{20}$ crystal: Simulation of Raman scattering

13:20 – 13:40 I. Piskunov *(Kharkiv, Ukraine)*
Methylammonium formate or a mixture of methylamine and formic acid: A challenge for classical molecular dynamics simulation

13:40 – 15:00 Lunch

Lviv Polytechnic National University, Main building,
Ju. Zachariewicz hall (room 214)

QUANTUM MATERIALS AND QUANTUM TECHNOLOGIES

Chaired by A. Kordyuk *(Kyiv, Ukraine)*

9:20 – 9:50 A.G. Sotnikov *(Kharkiv, Ukraine)*
Tensor network approach to study quantum many-body systems in three-dimensional lattices

9:50 – 10:20 L. Brizhik *(Kyiv, Ukraine)*
Long-range electron transport mediated by solitons in Donor–Alpha-Helix–Acceptor systems

10:20 – 10:50 T. Verkholyak *(Lviv, Ukraine)*
Low-temperature thermodynamics of the spin-1/2 Heisenberg model on the diamond-decorated square lattices within the classical monomer-dimer model

10:50 – 11:20 V. Pastukhov *(Lviv, Ukraine)*
Quantum-droplet phase of dilute BECs in the presence of disorder

11:20 – 11:40 Coffee break (room 231)

Chaired by A. Shvaika *(Lviv, Ukraine)*

11:40 – 12:10 Kh. Gnatenko *(Lviv, Ukraine)*
Studies of properties of evolutionary states of spin systems using quantum programming

12:10 – 12:40 V. Gerasimenko *(Kyiv, Ukraine)*
Dynamics of correlations in open quantum systems

12:40 – 13:00 T. Hutak *(Lviv, Ukraine)*
Flat-band Heisenberg antiferromagnet in a magnetic field

13:00 – 13:20 A. Shutovskyi *(Lutsk, Ukraine)*
Josephson junction dynamics with nontrivial current–phase relation

13:20 – 13:40 A.R. Kuzmak *(Lviv, Ukraine)*
Generation of spin interactions using laser radiation

13:40 – 15:00 Lunch

Lviv Polytechnic National University, Main building,
Matejko hall (Assembly hall)

Chaired by A. Belonoshko *(Nanjing, China)*

15:00 – 15:40 K. Wiesner *(Potsdam, Germany; online)*
Understanding regime changes using statistical physics: From deep neural networks to democratic nations

15:40 – 16:20 N. Lebovka *(Kyiv, Ukraine)*
Diffusion transport in 2D porous medium containing elongated obstacles

16:20 – 17:00 A. Honecker *(Cergy-Pontoise, France; online)*
Magneto-thermodynamics of the quantum Heisenberg model on simple cubic, square, and triangular lattices

17:00 – 17:20 Coffee break (room 231)

Chaired by L. Brizhik *(Kyiv, Ukraine)*

17:20 – 18:00 Y. Zolotaryuk *(Kyiv, Ukraine)*
Nonlinear localized modes in the classical *XY* model

18:00 – 18:40 V.M. Tkachuk *(Lviv, Ukraine)*
Quantum computation of the Ising model partition function

18:40 – 19:00 CLOSING CEREMONY

LIST OF POSTERS

1. O. Baran *(Lviv, Ukraine)*
   Magnetoelectric effect in a spin-1/2 XX sawtooth chain with three-spin interactions: Exact results

2. T. Demchuk *(Lviv, Ukraine)*
   Structural and collective dynamics in liquid Li along the 600 K isotherm: An *ab initio* molecular dynamics study

3. O. Derzhko *(Lviv, Ukraine)*
   Specific heat probes of quantum 3D Heisenberg magnets

4. O. Derzhko *(Lviv, Ukraine)*
   Simple model of magnetoelectric crystal. Dynamic properties

5. B. Dobosh *(Kyiv, Ukraine)*
   Active matter: From simulations of agent-based swarms to collective phases

6. O.A. Dobush *(Lviv, Ukraine)*
   Triple point in a cell model with Curie–Weiss-type interaction

7. O.A. Dobush *(Lviv, Ukraine)*
   Influence of microscopic parameters on phase behavior of a cell model with Curie–Weiss interaction

8. I. Gapyak *(Kyiv, Ukraine)*
   Kinetic evolution of an open system of hard spheres with initial correlations

9. K. Haydukivska *(Lviv, Ukraine)*
   Conformational transitions in stimuli responsive copolymer bottlebrushes: A dynamics study

10. Yu. Honchar *(Lviv, Ukraine)*
    Critical behavior and partition function zeros in decorated hierarchical lattices based on a triangle

11. O. Hryhorchak *(Lviv, Ukraine)*
Trimer–dimer transition in one-dimensional three-component fermions with three-body interaction

12. T. Hvozd *(Lviv, Ukraine)*
Modeling phase separation and percolation behavior in protein-regulator mixtures under crowding conditions

13. V. Ignatyuk *(Lviv, Ukraine)*
The recoherence/decoherence processes in a single qubit dephasing model

14. V. Ignatyuk *(Lviv, Ukraine)*
Ising model in the Rényi statistics: The finite size effects

15. J. Ilnytskyi *(Lviv, Ukraine)*
Interaction of colloidal particulates with microstructured thermo responsive polymer brush: computer simulations

16. O. Khomenko *(Sumy, Ukraine)*
Statistics of the self-affine regime of traffic flow

17. M. Kopcha *(Lviv, Ukraine)*
How different head groups affect binding of passivating ligands to $CsPbBr_3$ nanocrystals: Insights from atomistic simulations

18. M. Korvatska *(Lviv, Ukraine)*
Diffusion of hard-sphere mixture in disordered porous media from a new extended Enskog theory

19. P. Kostrobij *(Lviv, Ukraine)*
Modeling displacements of near-surface ionic layers in semi-infinite metallic systems

20. M. Krasnytska *(Lviv, Ukraine)*
From Zeros to Exponents: Critical and tricritical behavior in the Blume–Capel model on a complete graph

21. N. Kukarkin *(Lviv, Ukraine)*
Adsorption of disk-like particles on a patterned adhesive surface

22. V. Kulinskii *(Odesa, Ukraine)*
Some liquid–gas equilibrium regularities in view of global isomorphism approach

23. S. Kuzmin *(Odesa, Ukraine)*
Application of the zero-range potential model for calculation of electronic structure of molecules

24. V.O. Leonov *(Kyiv, Ukraine)*
Features of kinetics in a two-level system with time-dependent coupling to a boson field

25. A.F.C. Licha *(Potsdam, Germany)*
Numerical simulations to characterise phase transitions in the loss landscape of neural networks with L2 regularisers

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

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

28. A.V. Nazarenko *(Kyiv, Ukraine)*
Two-phase structure in the Bose–Einstein condensate dark matter model

29. I. Novoseltsev *(Kharkiv, Ukraine)*
Microscopic structure and energetics of Li+ ion solvation in benzonitrile: MD simulations vs. quantum chemistry calculations

30. G. Panochko *(Lviv, Ukraine)*
The dynamics of the spinful impurity in ideal Bose gas

31. M. Parymuda *(Lviv, Ukraine)*
Magnetothermodynamics of the antiferromagnetic Heisenberg model on the Tasaki lattice in an external magnetic field

32. Y. Perets *(Kyiv, Ukraine)*
Systematic investigation of density fluctuations in laser wakefield accelerators on the properties of the accelerated electrons

33. V. Polkanov *(Lviv, Ukraine)*
Bose condensate in low-dimensional bosons with three-body interaction

34. I.V. Pylyuk *(Lviv, Ukraine)*
Binodal and its diameter for Morse fluids near the critical point

35. R.V. Romanik *(Lviv, Ukraine)*
Entropy of a multiple-occupancy cell fluid model

36. P. Sakhniuk *(Lutsk, Ukraine)*
Modeling of distributions of the magnetic flux in long Josephson junctions with nontrivial current-phase relation

37. P. Sapriianchuk *(Lviv, Ukraine)*
Using word analysis to study single-file chain of water molecules in electric field

38. P. Sarkanych *(Lviv, Ukraine)*
Interaction topology effect on collective decision-making with heterogeneous biases

39. D. Shapoval *(Lviv, Ukraine)*
Reaction–diffusion processes in structurally heterogeneous media: A Monte Carlo study

40. R. Stetsiv *(Lviv, Ukraine)*
Structure factor and dynamic structure factor of one-dimensional ion conductors

41. M.V. Tokarchuk *(Lviv, Ukraine)*
Description processes of the interaction of water and aqueous solutions with fuel-containinig materials in the New Safe Confinement of the "Shelter" object

42. M.V. Tokarchuk *(Lviv, Ukraine)*
To the generalized equations of hydrodynamics for viscoelastic fluids in fractional derivatives

43. M.V. Tokarchuk *(Lviv, Ukraine)*
To the kinetic theory of dense gases and liquids. Calculation of quasi-equilibrium particle distribution functions by the method of collective variables

44. P. Trokhimchuck *(Lutsk, Ukraine)*
Role and place of classifications for the creation and the development of modern physics

45. A. Vdovych *(Lviv, Ukraine)*
Effect of electric field and mechanical stresses on thermodynamic characteristics of the NH_4HSO_4 ferroelectric within the framework of a two-sublattice pseudospin model

46. O.V. Velychko *(Lviv, Ukraine)*
Theory of a self-consistent local potential transformation for SPS-type ferroelectrics

47. V. Yanishevskyi *(Lviv, Ukraine)*
Path integral methods in stochastic equations

48. D. Yaremchuk *(Lviv, Ukraine)*
Thermoresponse of structured interface for cell sorting: DPD simulations study

The 6th Conference

"Statistical Physics: Theory and Computer Simulations"

Plennary Lectures

Abstracts

27–29 August 2025, Lviv, Ukraine

Hydrodynamic simulations and hydrodynamic limit of the scattering function via time-dependent non-equilibrium molecular dynamics

G. Ciccotti[a,b,c]

[a] *Istituto di Applicazioni del Calcolo, IAC-CNR, Rome, Italy*
[b] *Dipartimento di Fisica, Universita' di Roma "La Sapienza", Rome, Italy*
[c] *School of Physics, University College of Dublin, Dublin, Ireland*

The derivation of the hydrodynamic limit of the Van Hove function from a rigorous probabilistic approach is presented. Then, after recalling the extension of the standard stationary state (time averages!) Molecular Dynamics to time dependent non-equilibrium situations, we show how the same idea can be used to compute hydrodynamic relaxation processes. The procedure, which we have called Dynamical Non-Equilibrium Molecular Dynamics (D-NEMD), to distinguish it from the standard (stationary) NEMD, is based on a generalization of the linear response theory. The idea has been implicitly formulated by Onsager in the thirties in metaphysical language; has been given a solid statistical mechanical foundation in the fifties by Green and Kubo (in the linear and nonlinear regime); then has been proven useful in molecular simulation by the present author in collaboration with G. Jacucci and I.R. Mac Donald in the seventies. It has been called the nonlinear Kubo–Onsager relation. It permits to connect dynamical nonequilibrium averages or dynamical relaxations to the final stationary state (the chosen initial distribution, suitably sampled, is the key ingredient of the game). To show the power of the method we apply it to get the hydrodynamic relaxation of an interface between two immiscible liquids.

Searching for new quantum materials: Theory-guided approach with synchrotron ARPES

A.A. Kordyuk

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Quantum materials exhibit emergent phenomena with potential applications in next-generation quantum technologies. To accelerate their discovery, we apply a theory-assisted approach that integrates electronic structure prediction with synchrotron-based angle-resolved photoemission spectroscopy (ARPES). This synergy enables the identification of key spectral features associated with superconductivity, electronic ordering, and topological phases.

I will discuss examples including Fermi surface nesting in electronically ordered systems, high-temperature superconductivity in cuprates and iron-based superconductors, and the ongoing search for topological superconductivity. Particular attention will be given to machine learning models trained on synthetic ARPES spectra, which disentangle coherent and incoherent components and reveal interaction-driven features correlated with enhanced superconducting critical temperatures.

The talk will conclude with a perspective on the strategic importance of establishing a synchrotron facility in Ukraine to support advanced quantum materials research, foster international collaboration, and drive technological innovation.

This work is supported by the Federal Ministry of Research, Technology and Space (BMFTR) through the project GU-QuMat (grant number 01DK240008).

Statistical theory of charged particle systems including triple bound states — and the collaboration Lviv–Rostock*

W. Ebeling

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Honoring the hundredth anniversary of the birthday of Ihor R. Yukhnovskii we analyze new developments in the statistical thermodynamics of Coulombic systems. The basic idea of this work is to demonstrate that the exponential potential used in the first papers of Yukhnovskii is an appropriate reference systems for the description of charged particle systems. We briefly discuss the collaboration between the groups of Ihor R. Yukhnovskii in Lviv and Günter Kelbg in Rostock and analyze several approaches based on pair correlation functions and cluster expansion in the classical as well as in the quantum case.

Finally we discuss the progress in the statistical description of bound states of three particles as in helium plasmas and in $MgCl_2$-solutions in the classical case and present new results about the effects of three-particle bound states, in particular new expressions for the cluster integrals and the mass action functions of helium atoms and ionic triple associates.

*Dedicated to the memory of Ihor R. Yukhnovskii (1.09.1925–26.03.2024).

On the contribution of I. Yukhnovskii to the development of statistical theory of electrolyte solutions

M. Holovko

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I. Yukhnovskii started his activity in the statistical theory of electrolyte solutions nearly 75 years ago by modifying Coulomb interionic interaction due to strong repulsion at short distances. As a result, for the first time, it was possible to describe and to investigate the screening effects in electrolyte solutions for nonpoint ions. The obtained screening potentials were used for the formation of cluster expansions for the pair distribution functions of ionic systems in the framework of plasma parameter expansion and, after, in the framework of the collective variables approach. In the last approach it was possible also to include the short-range interactions explicitly. As a result, two different forms of cluster expansions were proposed, which were used for the investigation of electrolyte solutions. The first of them generalizes the Mayer density expansions for ionic systems, and in the second one, the subsystem with short-range interactions is considered as the reference system.

In the framework of obtained results, the ion-molecular approach was developed in the theory of electrolyte solutions, where solvent molecules together with ions are treated explicitly. As a result, it was possible to investigate the influence of ion–solvent and solvent–solvent interactions on the formation of effective interactions in solvent, the formation of different solvation structures in electrolyte solutions, and the treatment of cationic hydrolysis effects as the deprotonation of water molecules in the hydration shell of highly charged cations. Finally, the developed approach was generalized for the ion–molecular inhomogeneous case and used for the description of space-limited electrolyte solutions.

Fifty years of Yukhnovskii's critical point theory

J. Kozicki

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Half a century ago, professor Igor Yukhnovskii elaborated a method of studying the critical point of the three-dimensional Ising model based on the layer-by-layer integration in the space of collective variables. His technique was alternative to the ε-expansion method for which K.G. Wilson was awarded in 1982 by the Nobel Prize in physics. However, Yukhnovskii's technique — yielding similar results — provided even deeper insight into the nature of this phenomenon. At that time, we — professor's students — saw only this aspect of his theory. Later on, I realized that the mentioned Yukhnovskii's work fits naturally into a more general context of the turbulent development of quantum field theory and statistical physics in the last quarter of the twenties century. The aim of my talk is to show this.

Modeling of adsorption of water on solid surfaces chemically modified by grafting of chain molecules

O. Pizio

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Design of solid substrates with desired wetting properties is of much importance in materials science. One of successful experimental methods for this purpose is to graft chain molecules or polymers onto the smooth surface to form a brush-like structure. The wetting phenomena at such complex liquid-solid interface are determined by many competing factors. In the series of works [1–3], we have proposed and tested a theoretical approach corresponding to such setup. The method is a version of density functional technique for classical associating fluids. Specifically, our interest is in water in contact with graphite-like solid modified by grafted chain molecules. The method permits to obtain the adsorption isotherms and to construct the wetting phase diagrams. The growth of water film is explored. The results for the contact angle are compared with experimental data. Nontrivial dependence of the contact angle upon changes of geometric and energetic heterogeneity is observed. The effects of chains length and grafting density are investigated. Novel wetting phase behavior, due to changes of properties of bare solid surface upon grafting of chains, is observed and analyzed in view of possible applications.

1. O. Pizio, S. Sokolowski, J. Mol. Liq., 2023, 390, 123009.
2. O. Pizio, S. Sokolowski, J. Mol. Liq., 2022, 357, 119111.
3. O. Pizio, S. Sokolowski, Mol. Phys., 2022, 120:6, e2011454.

Molecular simulation of liquid crystals in periodic boundary conditions

M.P. Allen[a,b]

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In the nematic liquid crystal phase, the molecular orientational distribution is anisotropic. There is a preferred direction in space: the director $\mathbf{n}$, where $\pm\mathbf{n}$ are equivalent. Molecular orientations are distributed about this preferred direction. In macroscopic samples, the director is effectively fixed in space, or 'conserved', so spherical symmetry is broken, although (in the absence of external fields and surfaces) all director orientations are equally likely.

In finite-size molecular simulations, the director is not conserved, but typically varies only slowly. In spherical symmetry, all directions should be equally probable; however periodic boundary conditions reduce the symmetry. This means that, given adequate sampling, a non-isotropic director distribution might be observed, with some directions 'preferred' over others. It is even possible that the properties of the system (such as the nematic order parameter) could depend on the director orientation within the simulation box. In some early simulations of the nematic phase, truncated octahedral (TO) periodic boundaries were preferred to the more usual cubic (CB) periodic boundaries: it was conjectured that, being more 'spherical', they would have smaller effects on the nematic phase. Since there seem to be no reports of the observation of such effects, still less any attempts to systematically study them and quantify them, it may be that they are insignificant. Certainly, most simulators seem not to worry about them.

In this talk, I shall describe Monte Carlo simulations of a range of simple model molecular systems, at different system sizes, in the nematic phase, in both CB and TO boundaries. Each simulation is confined to a small window in the orientation space of $\mathbf{n}$. The results from a large number of overlapping windows are combined using the Multistate Bennett Acceptance Ratio method, to give the complete function $\mathcal{P}(\mathbf{n})$. This type of calculation turns out to be well-suited to a high-throughput ensemble-computing platform. Some early results will be presented, giving an idea of the extent to which the periodic boundaries affect the distribution.

Nonequilibrium Green functions simulations of femtosecond dynamics of quantum materials

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Finite two-dimensional quantum materials such as graphene nanoribbons of transition metal dichalcogenides offer unusual electronic properties such as strong electronic correlations, topological states and space dependent density of states. When these systems are excited by a short laser pulse, electronic and excitonic properties can be controlled on femtosecond time and sub-nanometer length scales [1]. I will describe how we model these systems and their dynamics using accurate nonequilibrium Green functions methods [2] which have recently accelerated tremendously [3,4].

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Impact of magnetism account on computation of iron phase diagram

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Iron (Fe) is a major component of the Earth and inhabited exoplanets cores, yet its phase diagram at extreme pressures (P) and temperatures (T) is a subject of extensive debate. Since the solid core is at the temperature close to melting it is of ultimate importance to know the structure of the sub–melting phase. Such knowledge enables understanding of the planet evolution from the beginning to the current state and predicting the future. While recent experiments provide the evidence for the stability of the body-centered cubic (bcc) phase, several theoretical studies point to the stability (even though marginal) of the hexagonal close–packed phase (hcp). None of those studies considered the itinerant magnetism of iron at extreme conditions. Here, we computed the melting curves using the density functional theory based molecular dynamics (DFT MD) with and without thermally induced longitudinal spin fluctuations (LSF). The non-magnetic DFT MD simulations result in stability of the hcp phase as the sub-melting phase with 8 and 16 valence electrons while the bcc phase stabilizes for the case of 14 valence electrons. The LSF DFT MD with 16 valence electrons favors the bcc phase stability. Therefore, we conclude that the account of magnetism results in the new physics of iron at extreme conditions and brings the theory in agreement with experiment as well as seismic data on the Earth Inner Core.

Stochastic population dynamics of competing species in driven and/or spatially inhomogeneous systems

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Agent-based Monte Carlo simulations of simple lattice models constitute a versatile tool to investigate stochastic population dynamics subject to time- and/or space-dependent rate parameters. I will address two topics: (1) To represent seasonal oscillations in resource availability, we implement a periodically varying carrying capacity in a two-dimensional Lotka–Volterra predator-prey model. We find that species coexistence is enhanced through this periodic drive. The fast- and slow switching regimes can be described through different effective static environments. Yet we observe intriguing resonant features when the external switching rate matches the internal population oscillation frequency, inducing persistent spatial correlations. (2) Stochastic population dynamics in finite systems often ultimately terminates in an absorbing state. However, in sufficiently large spatially extended models, the time to reach species fixation or extinction becomes exceedingly long, effectively permitting coexistence. Yet tuning certain control parameters, e.g., increasing the predation rate in predator-prey systems or enhancing asymmetries in cyclic dominance models, may render coexistence states in finite systems highly vulnerable against stochastic fluctuations. Intriguingly, though, they can be efficiently stabilized through continuous influx from the system's boundaries, which is generated via diffusive coupling of the vulnerable region to an adjacent stable patch. I will discuss (semi-)quantitative criteria that delineate the conditions for this remarkable boundary flow stabilization of finite-size absorbing-state instabilities in stochastic population dynamics with either cyclic or hierarchical competition.

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Using quantum computers to prepare ground states of the Hubbard model and in quantum chemistry

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In this talk, I will discuss the difference between a classical reservoir (which adds no additional quantum degrees of freedom) and a quantum reservoir (which does add quantum degrees of freedom). I will then explain why the classical reservoir is preferred for pure-state creation, because it cannot create mixed states. Then I will describe an efficient algorithm for ground-state preparation of the Hubbard model that avoids the need for Jordan–Wigner strings in the ansatz and just employs hopping terms and on-site correlations in preparing the ground state. I believe this is perhaps the nost efficient way to create ground states. I will also show how this approach compares to other methods for ground-state preparation such as couple-cluster approaches. I may even have some preliminary results for how well this methodology works in quantum chemistry ground-state preparation. The approach does require a global optimization strategy, which is complicated to implement, but this is ameliorated by the fact that the number of parameters can be kept rather small (empirically appearing to grow linearly with the number of sites/orbitals in the system). Our results have recently appeared in *Phys. Rev. B* **111**, 235152 (20025).
This work was completed in collaboration with Zach He, Lex Kemper, Lorenzo Del Re, and Dominika Zgid.

Multifractals in statistical mechanics

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The introduction of the concept of fractals, along with their associated fractal dimensions, allowed for the study of a large number of systems in statistical mechanics, both in and out of equilibrium [1].

However, other systems exhibited much more complex behavior, making it necessary to introduce the concept of multifractals, where many fractal structures coexist and a large number of fractal dimensions are needed to fully characterize their behavior. Multifractals can be found in turbulence, Anderson localization, surface growth, or the analysis of financial time series, to name just a few examples [2].

In this talk, we explore the multifractal properties of two key disordered systems: the 3D diluted Ising model (equilibrium) [3] and the 3D Edwards–Anderson model (out of equilibrium) [4]. Using extensive simulations on conventional clusters and on the Janus II supercomputer, we analyze the moments of the correlation function. Results for the diluted Ising model are compared with conformal field theory predictions [5], while for the 3D spin glass, we examine the impact of heterogeneity on glassy dynamics [4].

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4. M. Baity-Jesi et al. (Janus Coll.), *Multifractality in spin glasses*, *PNAS* **121** (2024) e2312880120.
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On the scaling properties of (2+1) directed polymers

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In this talk in terms of the replica method we consider both high and low temperature limit of (2+1) directed polymers in a random potential and propose an approach which allows to compute the scaling exponent θ of the free energy fluctuations as well as the left tail of its probability distribution function. It is argued that the values of θ are different in these two limits which implies that unlike the $(1 + 1)$ system in the two-dimensional case the free energy scaling exponent is non-universal being temperature dependent.

Mesoscopic theory for concentrated ionic systems

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Classical theories developed for dilute electrolytes are not valid when the average distance between the ions becomes comparable with their diameters. Unfortunately, different experimental techniques, approximate theories and simulations give contradictory results for the distribution of the ions and for screening of charged objects in concentrated ionic systems. Development of commonly accepted theory is important, because the density of ions in living cells is large, and concentrated ionic systems, including room-temperature ionic liquids, can find practical applications in energy storage devices.

I will very briefly present the experimental and simulation results. Next I will discuss major differences between dilute and concentrated ionic systems, and introduce the mesoscopic approach for ionic systems with any density. In the theory, the finite size of the ions and the variance of the local charge are taken into account. I will present correlation functions obtained within the theory on the level of the self-consistent Gaussian approximation. The results will be compared with experiments. I will also show the effect of charge ordering near an electrode on the capacitance. The remaining open questions will be discussed.

Biomolecular condensates and the physics of polymers in mixed solvents

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The discovery that many proteins—especially those with intrinsically disordered domains—can form temporary organelles, known as biomolecular condensates, through phase separation processes has fundamentally changed our understanding of biological functions. Central to these phenomena are phase transitions in complex polymer solutions, in which fundamental polymer properties—such as conformational transitions and the intrinsically low mixing entropy—play a key role. Many biomolecular condensates are formed through the co-condensation of proteins and polynucleotides, where at least one protein species preferentially interacts with RNA or DNA/chromatin. In most cases, the proteins that constitute the majority of the condensate exhibit a miscibility gap in aqueous solution at elevated concentrations in vitro. Recently, we proposed the theory of Polymer-Assisted Condensation (PAC), which predicts the formation of the condensate within the polymer's volume of gyration, where interactions with the three-dimensional conformation of the polymer trigger the phase transition of the protein component [1]. A key feature of these liquid condensates is their robustness against changes in parameters, as well as the dominant role played by the condensation free energy of the protein component. The formation and properties of heterochromatin, a genetically silenced region of eukaryotic chromosomes, can be explained by PAC, which resolves several issues present in previously published theories [2]. Recently, we developed a field-theoretic approach to PAC to better understand the adsorption and desorption scenarios of heterochromatin at the nuclear lamina [3].

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Collective dynamics in liquid water from computer simulations using molecular dynamics

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Collective effects in solids and liquids are an interesting topic of research that yields information about the structure and dynamics in materials [1]. The collective vibrational excitations in liquids are the corresponding counterpart to phonons in solids. They lead to effects such as the "fast sound" [2], where the velocity of the propagation speed of mesoscopic acoustic modes is clearly larger than expected from the macroscopic, hydrodynamic value of the adiabatic speed of sound.

Recently we investigated [3] the collective excitations in liquid water using density function theory-based molecular dynamics. We could derive the dispersion of the collective excitations and how the results qualitatively changed when the London dispersion forces were included.

Now we extend our former studies on the collective dynamics in liquid water by using recent models of interaction potentials, such as the `MB-pol` [4] and machine learning interaction potentials (MLIPs), such as a foundation model `MACE-OFF23` [5] and an explicitly fitted MLIP [6]. These allow us to perform longer simulations, with larger systems, thus allowing us attain better statistics and smaller wave vectors in the dispersion.

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Sagnac effect in graphene

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The Sagnac effect refers to the phase shift between two coherent waves, such as light, traveling in opposite directions within an interferometer mounted on a rotating disk. This principle forms the foundation of various modern navigation systems. Notably, laser gyroscopes based on the Sagnac effect are extensively employed in high-precision weapon. The magnitude of the phase shift is directly proportional to the area enclosed by the light rays, the frequency of the light, and the angular velocity of the interferometer's rotation. Given that material particles also exhibit wave-like properties, the Sagnac effect has been experimentally observed in free electrons in vacuum, neutrons, and even atoms. Moreover, when the Sagnac effect is realized on electrons, the resulting phase shift in the interference pattern is roughly a million times larger than that for light. This prompted a theoretical question: how would the Sagnac effect manifest in solid-state interferometers using free electrons in monolayer graphene? Graphene is known for its zero effective carrier mass and linear electron dispersion, properties that closely resemble those of light. We discovered that, despite these unique properties, the Sagnac effect in graphene is still governed by the mass of the free electron. As a result, the effect in graphene remains approximately a million times stronger than in light-based interferometers. The parameters of existing graphene samples make the practical realization of the Sagnac effect in graphene feasible.

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Understanding regime changes using statistical physics: From deep neural networks to democratic nations

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Statistical physics provides us with powerful tools to understand processes outside of physics. In particular, the study of complex systems benefits from the statistical viewpoint and the associated physics phenomenology. I will present two examples from my group's work. Example one is the transition from non-learning to learning in a deep neural network which exhibits the properties of a phase transition [1]. We explane this 'phase' transition in terms of geometric features of the 'model' space.

Example two is the transition from democratic to non-democratic or autocratic political regime types in the history of the 20th century [2]. We have explored and quantified these transitions using tools from the statistical physics of diffusion. I will present the results and link them to known historical events.

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Diffusion transport in 2D porous medium containing elongated obstacles

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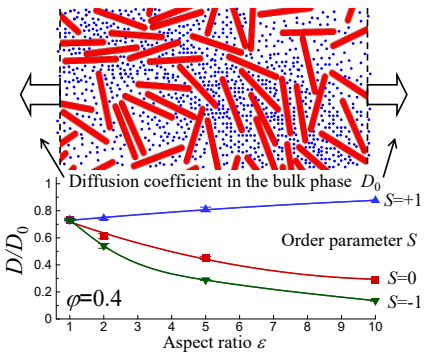
The constrained diffusion transport in two-dimensional slab containing elongated impenetrable obstacles (discorectangles) has been studied using the Monte-Carlo technique. The obstacles have discorectangle shape with aspect ratio ε = 1–10 and they are homogeneously distributed in systems with the surface coverage φ. The random walkers distributed inside the slab continuously extract to the external space outside of the slab.



Normalized diffusion coefficient D/D_0 versus the aspect ratio ε at different order parameters S.

The significant dependencies of diffusion coefficient D versus φ, ε and character of orientational ordering (order parameter S) are observed. For $S = -1$ or $S = 0$ an increase of aspect ratio ε resulted in decrease of diffusion coefficient D. It can be explained by formation of obstacle barriers for random walker movement. However, for obstacles ideally oriented perpendicularly to slab boundaries ($S = +1$) the opposite effects are observed. It this case obstacles supported the diffusion flow from the slab and an increase of ε resulted in increase diffusion coefficient D.

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Magneto-thermodynamics of the quantum Heisenberg model on simple cubic, square, and triangular lattices

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Many quantum-spin compounds realize a complex —typically higher-dimensional— exchange geometry. This poses a challenge for the theoretical description of their thermodynamic properties. Mean-field theory suggests itself as a flexible tool in this context. However, accuracy of simple single-site mean-field theory turns out to be disappointing for certain antiferromagnetic compounds with a low saturation field that are of potential interest for adiabatic demagnetization refrigeration [1]. We therefore revisit the mean-field approximation for the thermodynamic properties of the spin-1/2 Heisenberg ferro- and antiferromagnets on prototypical lattices such as the square, triangular, and simple cubic ones and benchmark it against numerical results obtained by quantum Monte Carlo simulations and exact diagonalization. Particular attention is paid to the magnetocaloric effect that constitutes the basis for adiabatic demagnetization refrigeration. In passing, we provide numerical reference data for thermodynamic properties of the spin-1/2 Heisenberg model on the simple cubic, square, and triangular lattices. We also discuss perspectives for improving the accuracy of mean-field methods.

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Nonlinear localized modes in the classical XY model

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It is shown that rotobreathers are generic solutions of the two-dimensional XY model with the nearest-neighbour interactions. Rotobreathers are periodic and spatially localized modes that cosist of several sites that rotate with some given frequency ω, while the rest of the lattice oscillates with the same frequency. The allowed range of the rotobreather frequencies begins from the upper edge of the linear spectrum Ω_π and continues to the arbitrarily large frequencies. Rotobreathers are linearly stable for the frequencies ω that satisfty the ineaquality $\omega > 2\Omega_\pi$.

Quantum computation of the Ising model partition function

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A key challenge in studying the thermodynamic properties of quantum systems and in computing their partition functions is that the Boltzmann factor is a non-unitary operator, while quantum computers operate using unitary transformations. We implement the Boltzmann factor for the Ising model on a quantum computer by expressing it as the trace of a unitary evolution operator, defined via an effective Hamiltonian, over ancillary qubits. This formulation establishes a bridge between unitary quantum evolution and the Boltzmann factor, enabling the computation of the partition function of the Ising model [1], including extensions with complex parameters. This approach allows for the investigation of Fisher and Lee–Yang zeros in the complex parameter space [2]. Furthermore, the same framework can be used to determine the ground state of a spin system, specifically, for the Ising model. As a demonstration, we calculate the partition function of a spin Ising cluster on an IBM quantum computer.

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The 6th Conference

"Statistical Physics: Theory and Computer Simulations"

Keynote Lectures

Abstracts

27–29 August 2025, Lviv, Ukraine

Modeling aggregation of amyloidogenic proteins by computer simulations

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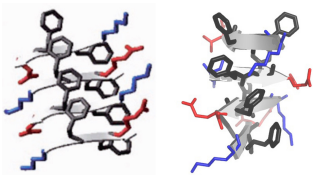

Protein aggregation refers to the process by which fully or partially unfolded proteins self-associate to make large and insoluble aggregates. A prominent example of the aggregates — amyloid fibrils is implicated in various neurodegenerative diseases and also has found multiple uses in technology. In this talk we will focus on what can be learned about amyloid formation using theoretical models and methods. First, we will give a broad overview of the problems and challenges facing theoretical approaches, ranging from the description of small oligomers [1], which are often considered kinetic intermediates to fibrils, continuing on to particlar details of amyloid structure [2]. Then, we will present a model — RAPID — specifically designed for simulation of protein aggregates [3,4] in water. Finally, we will discuss microscopic details of the aggregation pathway presented by the shortest amyloidogenic peptide reported so far — KFFE [1].

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Chelation of divalent heavy metal ions in aqueous environment

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The presence of heavy metal ions in aquatic environments poses a serious threat to human health, as these ions are highly toxic even at very low concentrations. Ethylenediaminetetraacetic acid (EDTA) and polyethyleneimine (PEI) are effective chelating agents capable of binding heavy metal ions to form stable complexes, thereby facilitating removal of the ions from aqueous solutions. We report our recent findings on the chelation of divalent heavy metal ions by two ligands: linear PEI [1] and EDTA [2]. Using molecular dynamics (MD) simulations under ambient conditions, combined with density functional theory (DFT) calculations, we investigate the structure and stability of the resulting ligand-ion complexes. We demonstrate that a linear PEI forms stable complexes with Hg^{2+} ions, with optimal stability found for chains containing five nitrogen units. For longer PEI chains composed of ten nitrogen atoms, a single PEI molecule can adsorb multiple ions, with stable complexes accommodating up to four mercury ions. For EDTA, we examine chelation complexes with Hg^{2+}, Cd^{2+}, and Pb^{2+} ions. Our results show that fully deprotonated EDTA exhibits the strongest binding affinity, while complexation efficiency decreases under acidic conditions. The structures of the observed complexes and the hydration shells of the considered ions are analysed in detail. This study provides atomistic insights into ligand-metal interactions and supports the rational design of PEI- and EDTA-based materials for wastewater purification.

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Topological resilience and thermodynamic signatures in virus–host interaction networks

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Understanding virus–host interactions is critical for anticipating the robustness of biological systems under perturbation. In this study, we examine molecular interaction networks between viruses and host species, using experimentally verified data from ViRBase v3.0. Focusing on *Homo sapiens*, *Mus musculus*, and *Gallus gallus*, we construct directed and undirected weighted graphs with nodes representing viral and host biomolecules (primarily miRNAs and proteins), and analyze their structural and dynamic properties.

We compute classical network parameters (such as degree distribution, density, betweenness, and assortativity), as well as thermodynamic-inspired metrics, including graph temperature and susceptibility, derived from spectral properties of the adjacency matrix and spin-based models. The stability of these networks is analyzed under two node-removal scenarios: targeted removal of highly central nodes and random node elimination.

Our results show that despite the removal of influential components, the networks maintain substantial connectivity, confirming their inherent robustness. The analysis reveals certain patterns in the dynamics of the calculated parameters. The behavior of graph susceptibility and magnetization suggests the presence of functionally critical nodes and motifs that govern global structural integrity.

By bridging network topology and thermodynamic analogies, we highlight new insights for interpreting virus–host interactions and identifying potential molecular targets for antiviral strategies. The observed irregularities in network degradation across removal strategies also emphasize the necessity for refined, context-aware approaches to biological network analysis.

Criticality of structurally-disordered spin systems with weak long-range interactions

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Studies of low-temperature ordering in long-range interacting many-particle systems attract continuing interest. Such systems are common in nature, but some features of their critical behavior still remain unexplained. We focus on the weak long-range interactions, decaying in a d-dimensional space as $x^{-d-\sigma}$ with $\sigma > 0$. In our study we address a challenging issue of a combined impact of weak structural disorder and weak long-range interactions on the critical behaviour in classical spin models. We review results obtained so far for the weakly diluted (random) long-range interacting n-vector model and provide new estimates of its critical behaviour. To this end, we apply the field-theoretical renormalization group approach refined by the resummation of diverging perturbation theory series. It is well established that the model describes the emergence of a new "random long-range" universality class for the specific region of the parameters (n, d, σ). To quantify its features we calculate marginal dimensions and critical exponents that govern criticality in the new universality class [1]. We compare results of the $\epsilon' = 2\sigma - d$-expansion and those obtained analyzing renormalization-group functions at fixed d, σ and discuss the convergence properties of resulting perturbative expansions.

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Topology-driven self-assembly in cyclic polymers

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Topological modification of block copolymer (BCP) conformations offers a promising approach for developing self-assembled periodic nanostructured materials with smaller domain sizes, which are essential for a range of technological applications. Cyclic polymers, with their inherently more compact conformations, present an effective strategy for achieving this miniaturization. Through a combination of analytical theory and coarse-grained molecular dynamics simulations, we establish a relationship between different nonlinear topologies and the corresponding domain size of lamella-forming BCPs. Our investigations includes BCP architectures with one or two cyclic segments such as tadpoles, diblock and triblock 8-shaped polymers, and diblock non-concatenated and concatenated rings.

We demonstrate that the primary reduction in lamellar domain size is driven by the more compact arrangement of monomers in the cyclic architectures, with an additional contribution from the non-concatenation of cyclic segments. This is corroborated by theoretical predictions for both domain size reduction and BCP conformations across different architectures.

Electrical conductivity of DNA-counterion systems: theory and computer simulations

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The DNA macromolecule is one of the most important molecules of life. Due to its biological significance, studies of its physical properties are often closely linked to its biological functions. However, the global abundance of DNA, which is comparable to that of oil, also makes it a promising material for practical applications. In this context, exploring various physical properties of DNA becomes relevant not only from a biological perspective but also for potential technological uses. Among the wide range of applications envisioned for DNA-based materials, one of the most intriguing and speculative is the use of DNA as a nanoscale wire. In this regard, the question of its electrical conductivity becomes crucial.

The conductivity of DNA can be considered from two perspectives. The first is intrinsic conductivity, which may arise from the electronic structure of the DNA itself. This type of conductivity can be particularly pronounced in the case of metalized DNA, where metal ions (such as Ag^+) are incorporated into the interior of the double helix [Kondo J. *et al.* Nat. Chem. 2017, 9 (10), 956–960]. The inclusion of metal ions within the DNA structure imparts novel electronic properties to the system, which are still not fully understood.

The second type is ionic conductivity, which arises from the motion of metal counterions that condense around the negatively charged DNA macromolecule. Molecular dynamics simulations have shown that the mobility of these counterions is influenced by the structural features of the DNA double helix [Zdorevskyi O.O. and S.M. Perepelytsya, Eur. Phys. J. E, 43, 77 (2020)]. This structural modulation of ion dynamics may play a key role in determining the electrochemical behavior of DNA-based systems, making them promising for various technological applications — for instance, in the development of DNA-based electrical supercapacitors [Mitta S.B. *et al.* Adv. Mat. Interf. 2022, 9 (14)].

This presentation will provide an overview of the current state of research in both areas.

Microscopic structure, solvation and transport properties of LiFSI and LiFTFSI in EMC and NDF solutions: MD simulation

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Lithium-ion batteries (LIBs) are one of the key technologies of modern energy. One of the most critical elements of the LIBs is the electrolyte, which control both Li^+ transport and interfacial reaction. Traditional electrolytes based on liquid organic solvents, although exhibiting high ionic conductivity, have certain drawbacks, such as low thermal stability and susceptibility to degradation at high temperatures. Therefore, the development of new types of electrolytes is a pressing task to improve the characteristics of LIBs [1].

In this contribution we present the results of molecular dynamics simulations of 1M solutions of Lithium (Fluorosulfonyl) (trifluoromethanesulfonyl)-imide (LiFTFSI) and Lithium bis(fluorosulfonyl)imide LiFSI in Ethyl methyl carbonate (EMC) and N,N-diethyl-trifluoromethane-sulfonamide (NDF) at −40, RT and 80 °C. The force filed for all the particle were generated by using the combination of LigParGen [2] intramolecular and short range intermolecular potentials and partial charges calculated at the M062X/AUG-cc-PVTZ/ChelpG level. The microscopic structure of the investigated electrolyte was analyzed in terms of radial distribution functions (RDF) and the running coordination numbers (RCN). We found that lithium coordinates around itself 3 FSI^- anions and 2 $FTFSI^-$ anions and approximately 3 solvent molecules. Variation in microscopic structure as a function of anion and solvent nature is addressed in terms of competition between inter-ion and ion-molecular interactions. The influence of temperature on ion solvation and diffusion also discussed.

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Electric field effects on the quasiphase transition of confined water in single-wall carbon nanotubes

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Recent studies [1,2] have shown that water molecules encapsulated in (6,5) single-wall carbon nanotubes (SWCNT) undergo a temperature-induced quasiphase transition, governed by changes in the balance of intermolecular interactions resulting in altered orientational ordering of dipoles. In our previous work [3], a comprehensive theoretical analysis of this phenomenon is performed using quantum chemical calculations, molecular dynamics simulations, and a simplified lattice model. Such an approach accounted for both short- and long-range interactions as well as rotational constraints imposed by the nanotube geometry, successfully reproducing the orientational behavior observed experimentally. By engaging the above trio of quantum chemistry, molecular dynamics simulations, and lattice model in the continuation study, we explore the influence of external electric fields (with strengths up to 10^8 V/m) directed along the SWCNT axis on the confined water. The results reveal a significant field-induced modulation of the quasiphase transition: the temperature at which the tangential component of the total dipole moment of water reaches its maximum is shifted upward, indicating stabilization of the intermediate ordered phase. Moreover, the angles between water dipoles and nanotube axis are reduced under stronger fields, hence promoting the axial polarization of the water chain toward higher temperatures. These findings suggest that electric fields can effectively tune the orientational ordering and thermodynamic behavior of confined water, with implications for nanoscale fluid transport, sensing, and energy conversion applications.

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Coagulation-flocculation process on a lattice: Monte Carlo simulations

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We consider a coarse-grained modelling approach to the coagulation-flocculation processes related to wastewater purification schemes. A non-trivial DLA (diffusion-limited aggregation) of N_{DLA} particles, representing impurities in solvent is considered, with the particle coagulation probability $0 \leq p \leq 1$ ($p = 1$ recovers standard DLA). Linear polymeric flocculant, considered as a "seed" for DLA process, is modelled via the self-avoiding walk (SAW) of N_{SAW} monomers, Flocculation occurs by adsorbing diffusive particles of the DLA by monomers of polymer seed, the process is irreversible with the probability equal to one. Coagulation and flocculation occur simultaneously with the ratio between their dynamics defined by the value of p. Within the frames of computer simulations on a square dimensional lattice, we focus on the evaluation of parameters as: (i) adsorbing efficiency N_a of SAW, characterized by the averaged number of impurities adsorbed directly on its perimeter; (ii) the effective size of coagulation-flocculation (DLA-SAW) aggregate, as given e.g. by its gyration radius $R_{g\mathrm{DLA-SAW}}$; and (iii) the fractal dimension of such aggregates. These are studied within a wide range for each parameter from a set $\{p, N_{\mathrm{DLA}}, N_{\mathrm{SAW}}\}$.

Computer simulations of adsorption of low density lipoproteins on a photosensitive polymer brush

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One of the strategies to reduce the contents of low density lipoproteins (LDLs) in blood is a hemoperfusion, when they are selectively retracted from plasma by an adsorber located outside the patient's body. Recently, a photo-controllable smart surface was developed characterized by high selectivity and reusability [1]. It comprises a nanocarrier functionalised by a brush of azobenzene-containing polymer chains. We present a mesoscopic model for such a setup, and focus on the effects of molecular architecture and molecular weight of the polymers, as well as their grafting density, on the adsorption efficiency. The main mechanism of adsorption is attraction between phospholipids and *trans*-azobenzenes, both hydrophobic. The model system is studied via coarse-grained molecular dynamics simulations mimicking relevant atomic groups by soft-core beads. Adsorption efficency is characterized via binding energy of a single LDL to the brush structure. Most results are obtained for the case of linear chains, and adsorption efficiency is found to be the result of the competition between the simultaneous concentration of azobenzenes and phospholipids in the same spatial region, flexibility of polymer chains, and associated excluded volume effects [2]. Preliminary simulations obtained for the case of the brush made of center-grafted star-like polymers indicate that it can be more efficient as the LDL adsorber, comparing to the brush of linear chains, in a certain range of the brush parameters. Supported by NRFU grant 2023.05/0019.

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Tensor network approach to study quantum many-body systems in three-dimensional lattices

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Three-dimensional lattice systems are a fact of our everyday experience, since they are the natural building blocks of quantum materials. They became an excellent platform for the development and application of the beyond-mean-field approaches, which are capable of capturing the non-trivial quantum entanglement phenomena and, in particular, the topological order. Tensor networks are one of the most powerful and accurate approaches in this direction.

Calculation of observables with the representation of the many-body wave function in the form of three-dimensional projected entangled pair states is generally hard, as it requires a contraction of complex multi-layer tensor networks. We utilize the multi-layer structure of these tensor networks to largely simplify the contraction. The proposed approach involves the usage of the layer structure both to simplify the search for the boundary projected entangled pair states and the single-layer mapping of the final corner transfer matrix renormalization group contraction [1]. We benchmark our results on the cubic lattice Heisenberg spin-1/2 model and find a good agreement with the previous results.

Furthermore, we extend our approach to study the SU(4)-symmetric Heisenberg model on anisotropic cubic lattice. We show that, as the accuracy controlled by the bond dimension increases, the system forms a Néel-type ordering of dimers, in contrast to predictions of the mean-field approaches and in agreement with previous findings for the SU(4)-symmetric Heisenberg model on the square lattice.

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Long-range electron transport mediated by solitons in Donor–Alpha-Helix–Acceptor systems

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It is known that Davydov solitons [1] provide the long-range electron transport in an isolated one-dimensional molecular chain. Such a soliton is a bound state of a quasiparticle and local deformation of the chain formed due to the electron-lattice interaction. Here the results are reported on the study of the long-range electron and energy transfer mediated by solitons formed in an alpha-helical three-spine polypeptide coupled to donor and acceptor molecules at opposite ends [2]. It is shown that there exists the broad interval of the parameters for which an electron initially located on the donor, tunnels onto the chain where it forms a solitoocated on the donor, tunnels onto the chain where it forms a soliton-like state, which then travels to the opposite end, where it is captured by the acceptor. It is shown that the efficiency of the electron transport from the donor to the acceptor can reach 90%.

These results explain highly efficient long-range donor-accepor electron transport in redox reactions in photosynthesis and cellular respiration in biological systems, and in donor-acceptor systems mediated by various types of long molecular chains, widely used in modern microelectronics and nanotechnologies [3].

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Low-temperature thermodynamics of the spin-1/2 Heisenberg model on the diamond-decorated square lattices within the classical monomer-dimer model

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We explore the spin-1/2 Heisenberg antiferromagnet on diamond-decorated lattices to analyze their complex quantum phases and thermodynamic properties under a magnetic field [1,2]. Our study is focused on the dimer-tetramer phase which is characterized by the short-range correlations and localized singlet states either on diamond decorations or on dimers. The dimer-tetramer phase on the uniform and isotropic lattices shows the macroscopic degeneracy in the ground state. Its low-temperature thermodynamics can be effectively described by the classical monomer-dimer models on their respective lattices without diamond decorations. We study the enhanced magnetocaloric effect in the region of the dimer-tetramer phase for the spin-1/2 Heisenberg model on the diamond-decorated square lattice. In addition, the models on the non-uniform diamond-decorated square and honeycomb lattices are also considered to reveal the possible Kasteleyn-like phase transition in the effective dimer models on the corresponding lattices.

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Quantum-droplet phase of dilute BECs in the presence of disorder

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The equilibrium ground-state properties of quantum droplets in dilute Bose-Einstein condensates with the quenched Gaussian δ-correlated disorder are discussed. In particular, we have considered quantum droplet states in the three-dimensional two-component Bose systems and the one-component quasi-one-dimensional Bose gases with dipolar interaction between atoms. In both cases, the interplay between disorder and effects of the quantum fluctuation drastically changes the phase diagram of the system, leading to the emergence of thermodynamically stable large quantum droplets with two distinct densities. Higher-density structures are shown to be more energetically preferable. Peculiarities of the finite-size quantum droplets are extensively outlined in both approximate analytical and numerical calculations. Finally, we briefly discuss a possible experimental verification of the obtained results.

Studies of properties of evolutionary states of spin systems using quantum programming

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The rapid recent development of quantum technologies has opened up the possibility to study the properties of quantum systems and their states using quantum programming. We consider spin systems described by the Ising model that are one of the most suitable systems for modeling them on a quantum computer.

The entanglement distance of the system's evolutionary states has been calculated analytically. We have found find its dependence on the interaction coupling constants and the parameters of the initial state. In addition, the energy fluctuations and quantum correlators are calculated analytically as well as with quantum programming [1]. Specific cases of spin systems are considered as examples, including a two-spin system and spin chains. The results of quantum computing are in agreement with the theoretical ones.

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Dynamics of correlations in open quantum systems

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In quantum information theory, the evolution of a system is described by a quantum channel, which pertains to open quantum systems. This lecture will focus on the evolution of open quantum systems, i.e., quantum systems that interact with an external environment. We will review a novel method for describing the collective behavior of these systems based on the evolution of correlations [1–3].

One major advantage of this approach is that it allows us to derive a master equation that incorporates the initial correlations of particle states within an open system, particularly those that define their entangled states. This method also allows us to describe the decoherence processes in open quantum systems through kinetic equations that include initial correlations. Additionally, it addresses to the challenge of rigorously deriving the non-Markovian master equation, which generalizes the Fokker–Planck kinetic equation and accounts for memory effects in quantum systems interacting with their environments.

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The 6th Conference

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Abstracts

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Linking diffusion to cyanide biodegradation kinetics

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We present a comprehensive theoretical framework linking cyanide diffusion through bacterial outer membranes to biodegradation kinetics in gram-negative bacteria. Our analysis focuses on the transport of various cyanide compounds (free cyanide CN^-, thiocyanate SCN^-, and metal-cyanide complexes like $[Ag(CN)_2]^-$, $[Fe(CN)_6]^{3-/4-}$, etc.) through general porins OmpF, OmpC, OmpA, and OprF, and establishes quantitative criteria for determining when biodegradation becomes diffusion-limited [1]. The diffusion process is significantly influenced by electrostatic effects, particularly the Donnan potential across the outer membrane which creates strong selectivity against negatively charged cyanides. For instance, based on our calculations, $[Ag(CN)_2]^-$ exhibits substantially higher permeability than $[Fe(CN)_6]^{4-}$, correlating with experimental observations of their relative impact on bacterial respiratory activity [1].

We introduce a novel procedure based on the Goldman-Hodgkin-Katz flux equation to quantify when cyanide biodegradation transitions from a kinetically-controlled to a diffusion-limited process [1]. The key parameter is the ratio $\Delta C_{\text{in}}/C_{\text{in}}^{\text{eq}}$, where ΔC_{in} represents the concentration difference between equilibrium $C_{\text{in}}^{\text{eq}}$ and steady-state concentrations in the periplasmic space. When this ratio is negligible (< 0.05), diffusion is significantly faster than biodegradation, enabling model simplification.

This approach allows transition from complex multi-compartment models considering both extracellular and periplasmic cyanide concentrations to simplified kinetic models based solely on measurable extracellular concentration. Applied to experimental studies with *P. fluorescens* and *P. pseudoalcaligenes*, we demonstrate that diffusion remains significantly faster than biodegradation across typical concentration ranges, validating the use of simplified Michaelis–Menten kinetics in terms of extracellular cyanide concentrations [1]. These findings provide theoretical foundations for optimizing biological cyanide treatment processes.

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A model for the effective dielectric response of granular mixtures

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We present a model to calculate the effective quasistatic complex permittivity $\varepsilon = \varepsilon' + i\varepsilon''$ of a macroscopically homogeneous and isotropic mixture of fine solid grains with complex permittivity tensor ε_{ik} that are embedded in a uniform host. The permittivity ε is determined as the proportionality coefficient in the linear constitutive equation between the average complex electric current $\langle \mathbf{J} \rangle$ and electric field $\langle \mathbf{E} \rangle$ in the mixture. These averages are calculated using (a) the compact group approach [1,2] and (b) requirement [3] that the standard boundary condition of electrodynamics remain valid for all (including imagined) systems involved in the homogenization algorithm.

Within (a), the mixture is viewed as a set of macroscopic regions (compact groups) that are small compared to the wavelength λ of probing field in a medium they are imagined to be in, but that contain sufficiently many grains to retain the properties of the entire mixture. In the limit $\lambda \to \infty$, compact groups can be taken to be large enough to neglect the between-group correlations. At the same time, they can still be considered as point-like inhomogeneities when compared to λ. Using the theory of distributions, their contributions to $\langle \mathbf{J} \rangle$ and $\langle \mathbf{E} \rangle$ are extracted from all terms in the corresponding iterative series without detailed assumptions about many-particle effects inside compact groups. Requirement (b), on its part, leads to the conclusion that from among different types, it is the Bruggeman-type homogenization that is compatible with (a) and must thus be used to close the problem.

The equation for ε is obtained in terms of ε_{ik} by summing up the statistical moments for the deviation of the complex permittivity distribution in the system from ε. It is rigorous for static fields and, in particular, recovers the famous results for ε' of dilute mixtures of uniaxial spheres (Levy and Stroud) and ε'' of polycrystals (Hashin and Strikman).

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Polymerizing hard spheres with double shielded attractive shell

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We propose a model of polymerizing hard spheres with double square-well bonding potential. The model is represented by the equimolar two-component hard-sphere mixture with hard spheres of the same size σ. In addition to the hard-sphere repulsion particles of different species interact with double square-well potential with two binding minima located at a distances $0 < L_s < L_l < \sigma$. The structure of aggregates formed depends on the values of the bonding distances L_s and L_l. For $L_s, L_l < \sigma/2$ the particles can form only dimers with two bonding length, for $L_s < \sigma/2$ and $\sigma/2 < L_l < \sigma/\sqrt{3}$ each particle can form either one bond of the length L_s or two bonds of the length L_l , thus the aggregates formed will be represented by the dimers with bonding distance L_s and chains with the bonding distance L_l. Theoretical description of the model is carried out using extension of resummed thermodynamic perturbation theory [1,2]. We calculate thermodynamic and aggregation properties of the model and results compare against corresponding computer simulation results. Very good agreement was observed. Our analysis demonstrate highly nontrivial aggregation behavior of the model due to competition of bonding at two different distances, i.e. L_s and L_l. With appropriate choice of the potential model parameters (the depths and widths of its wells) two scenarios of the temperature dependence of the type of clusters formed was observed. According to the first one upon decreasing the temperature the system first form dimers with bonding length L_s. Further decrease of the temperature destroys dimers and form instead linear chains with bonding length L_l. According to the second scenario the system first form linear chains, which are destroyed in favor of dimers upon additional temperature decrease. This unusual behavior offers a possibility to manipulate the type of the clusters formed via external stimuli. Upon either increasing or decreasing the temperature the system can be driven to form ordering observed in liquid crystals.

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Spontaneous pattern formation in mixtures with competing interactions

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We will present the theoretical and simulation results for binary mixtures with competing interactions leading to spontaneous pattern formation. We focus on generic 3D and quasi-2D models of binary mixtures. In these models, like particles interact with short-range attraction long-range repulsion (SALR), and cross-interaction is of opposite sign. The models are inspired by effective interactions in biological or soft-matter systems. Using the mesoscopic theory, we obtain the phase diagrams for several versions of the above potentials in mean-field approximation and with the effect of fluctuations taken into account. The results are verified by MC and MD simulations. We obtain self-assembly into alternating layers of the first and the second component, and hexagonal arrangement of clusters of the minority component in the liquid of the majority component. Different shapes of the above interactions lead mainly to different size of the aggregates, and to some differences in fine details of the ordered patterns. In the considered mixtures, ordered phases are stable up to much higher temperature than in one-component systems.

A novel approach to the reference equation of state for real fluids

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The development of liquid-state theories, as well as the modeling of fluid behavior for industrial applications, requires accurate reference equations of state in closed analytical form. For decades, the cubic and generalized cubic van der Waals equations of state have played a central role in this field. However, these models are often inadequate due to their limited flexibility in certain thermodynamic regimes and their lack of a rigorous theoretical foundation.

Over the past fifteen years of research in this area, we have come to recognize that the conceptual framework introduced by van der Waals — particularly his distinction between two types of attractive forces, one contributing to surface pressure and the other to internal pressure, as outlined in his 1910 Nobel lecture — has been largely overlooked in modern statistical physics of the liquid state.

The purpose of this lecture is to: (i) revisit and highlight these important but neglected ideas of van der Waals; (ii) demonstrate the key implications of incorporating them into modern theory; (iii) present a novel equation of state in closed analytical form for a simple pure substance; and (iv) briefly discuss its extension to complex fluids.

Breakdown of hydrodynamics in a one-dimensional cold gas

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We consider the following one-dimensional alternating hard particle cold gas model: a set of point particles with alternating masses $m, \mu, m, \ldots$, with $m \geq \mu$ is distributed over the positive half-axis $x \geq 0$. Their dynamics is initiated by giving unit velocity in the positive direction to the particle located at the origin; in its course the particles undergo elastic collisions. An inherent feature of such a billiard is the emergence of two different modes that characterize its dynamics: the shock wave that propagates in $x \geq 0$ and the splash region in $x < 0$ [1]. As has been shown in [1], when the particle initial locations are random and uniformly distributed, the motion of the shock wave front $\mathcal{R}(t)$ is governed by hydrodynamics equations and its asymptotics at large times t is $\mathcal{R}(t) \sim t^{\delta}$ with $\delta < 1$. Whereas the splatter — the particles with locations $x \leq 0$ — moves in the ballistic way and eventually takes over the whole energy of the system.

In this study we demonstrate how the above hydrodynamic picture is violated when the initial particle locations are non random. By explicit analytical calculations we show that at certain ratios of particle masses $\mathcal{M}_i = m/\mu$ the splatter is absent and the front moves rightward in a ballistic way. We explicitly calculate first several hundreds $\mathcal{M}_i$ and support our findings by extensive molecular dynamics simulations [2]. For the mass ratios $m/\mu \neq \mathcal{M}_i$ our results [3] confirm findings of [1].

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Geometry of learning: L2 phase transitions in deep and shallow neural networks

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When neural networks (NNs) are subject to L2 regularization, increasing the regularization strength beyond a certain threshold pushes the model into an under-parameterization regime. This transition manifests as a first-order phase transition in single-hidden-layer NNs and a second-order phase transition in NNs with two or more hidden layers. We investigate a framework for such transitions by integrating the Ricci curvature of the loss landscape with regularizer-driven deep learning. First, we show that a curvature change-point separates the model-accuracy regimes in the onset of learning and that it is identical to the critical point of the phase transition driven by regularization. Second, we show that for more complex data sets additional phase transitions exist between model accuracies, and that they are again identical to curvature change points in the error landscape.

Olfactory receptor neuron stimulated with Markov process

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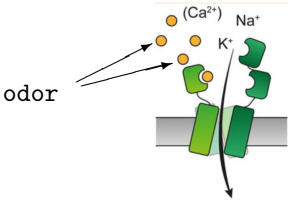
Excitable membrane of olfactory receptor neuron (ORN) is populated with large number of identical receptor proteins (**R**) able to bind/release odor (**O**) molecules. Affinity between **R** and **O** depends on the odor presented, and this is the very first mechanism enabling olfactory selectivity.

Our aim is to compare the **R** selectivity, expressed in terms of affinity, with that of ORN, expressed in terms of its firing rate. For this purpose we model the number of **R** bound with **O** at time t, $n(t)$, as a Markov stochastic process. With each bound **R**, as it is observed for insects, we associate an open channel having conductance 0.015 nS, which injects a depolarizing current through the membrane (see a figure above). The ORN's membrane voltage is governed by the leaky integrate-and-fire neuronal model, see an equation below:



Simplified **R** structure (modified from 10.1007/s00441-020-03363-x).

$$c_M \frac{\mathrm{d}V(t)}{\mathrm{d}t} = -g_l(V(t) - V_{rest}) - n(t)g_R(V(t) - V_e),$$

where $V(t)$ is the membrane voltage; V_{rest} is the resting voltage; c_M is the total capacity of ORN's membrane; g_l is the total leakage through it; V_e is the reversal potential for current through an open **R**; $n(t)$ is the fluctuating number of open channels at moment t due to odor molecules bound with **R**; g_R is the conductance of a single open channel. The total number of **R** per ORN is $N = 2.5 \cdot 10^6$ (the number observed for moth).

By means of numerical simulation of the Markov process $n(t)$ and the aforementioned equation we conclude that the ORN selectivity can be much better than that of its receptor proteins **R**. The effect of the selectivity gain is better pronounced if odors are presented at low concentration.

Application of Langevin dynamics for stochastic optimization in machine learning

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In this talk we demonstrate that optimization process of a machine learning model can be described by Langevin dynamics of a (virtual) Brownian particle with unit mass $m = 1$ in the space of trainable parameters $\theta \in \mathbb{R}^N$. The particle is subject to stochastic force, calculated as a negative stochastic gradient of the loss function $\hat{f} = -\nabla_\theta \hat{U}$. Therefore, the corresponding discrete-time Langevin equation is as follows:

$$\frac{\Delta\theta_{n+1} - \Delta\theta_n}{\Delta t^2} = \hat{f}_n - \gamma \frac{\Delta\theta_{n+1} + \Delta\theta_n}{2\Delta t},$$

where n is an iteration number, $\Delta\theta_{n+1} = \theta_{n+1} - \theta_n$, Δt is a time step and $\gamma > 0$ is a viscous friction coefficient. From the aforementioned Langevin equation, it is straightforward to obtain the next parameter updating formula:

$$\Delta\theta_{n+1} = \rho\Delta\theta_n + \hat{f}_n \cdot \eta,$$

where $\rho = (1 - \gamma\Delta t/2) / (1 + \gamma\Delta t/2)$ is conventionally called a momentum coefficient and $\eta = \Delta t^2(1 + \rho)/2$ is a learning rate constant. To implement simulated annealing (or slow cooling, in physical terms), we apply a certain schedule for the gradual momentum coefficient decrease in the range $0 \le \rho < 1$. Here we demonstrate that application of Langevin dynamics with simulated annealing to stochastic optimization tasks gives promising results in artificial intelligence [1], quantum computing [2] and optical engineering [3].

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Stochastic dynamics of magnetic textures on the racetrack memory

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Domain wall or skyrmion-based racetrack memory devices are formed from nanostripes that have three main components: (i) write ports, which involve the creation and movement of magnetic textures, (ii) a bit storage (cache), and (iii) read ports. One of the main technological challenges in racetrack memory is to achieve the highest possible packing density of nanoscale magnetic textures and, at the same time, the ability to read domain walls (or skyrmions) when they are tightly packed together [1]. Understanding the stochastic processes that affect the stable operation of new magnetic memory devices is crucial. Such randomness can be caused by noise of various natures, for example, thermal (equilibrium) or current (non-equilibrium) fluctuations. A key question that needs to be addressed is how perfectly the domain wall or skyrmion motion can be controlled under such conditions.

We present a theoretical description of the contribution of both equilibrium and non-equilibrium fluctuations to the stochastic dynamics of domain walls and skyrmions in racetrack memory. We consider two forms of the stochastic Landau–Lifshitz–Hilbert equations, which include spin-transfer and spin-orbit torque. Both equations simultaneously take into account the temperature-dependent thermal noise term and the spin current noise. The calculation of the diffusion matrices for the domain wall and skyrmion is performed using the Thiele analytical approach. Our theoretical results are independently verified by micromagnetic simulations using the COMSOL Multiphysics® software and the public code mumax3.

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Absence of a boson peak in low-temperature heat capacity of some layered materials

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In many disordered or amorphous materials, the low-temperature heat capacity exhibits an excess contribution compared to the Debye model prediction, known as the boson peak. This anomaly in the vibrational density of states (VDOS) is typically observed in C/T^3 vs. T plots and is strongly associated with disorder, structural inhomogeneity, or glass-like behavior. The boson peak is a well-documented feature in non-crystalline solids; however, calorimetric studies on layered solids, such as carbon polymorphs and disordered molecular systems with specific 2D stacking, have reported its absence in low-temperature heat capacity measurements.

This absence suggests that these materials do not exhibit the same low-energy phonon anomalies commonly seen in amorphous systems, indicating a more well-ordered phonon spectrum with no significant excess in low-frequency vibrational modes beyond what is expected from standard phonon dispersion relations. Several factors may contribute to this behavior. Layered materials exhibit strong in-plane bonding and weak van der Waals interlayer interactions, resulting in highly anisotropic phonon dispersion. Furthermore, the presence of a negative C_5T^5 contribution in the low-temperature heat capacity suggests the dominance of flexural phonon dispersion, further reinforcing the absence of the boson peak. This finding challenges conventional assumptions about phonon dynamics in reduced-dimensional systems and provides new insights into the fundamental thermal and vibrational properties of layered materials.

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Lattice dynamics of $Bi_{12}SiO_{20}$ crystal: Simulation of Raman scattering

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We present a combined theoretical and experimental study of the lattice dynamics of the $Bi_{12}SiO_{20}$ crystal. Using a first-principles approach, we calculated the phonon spectrum of this crystal at the Γ point and along the symmetry directions of the Brillouin zone. All phonon modes were classified according to the irreducible representations of the cubic I23 group.

Polarized micro-Raman spectra were measured in an oriented single crystal. Since phonon modes of the A and E types cannot be separated in Raman scattering of $Bi_{12}SiO_{20}$, a special experimental technique was used to determine the frequencies of A and E modes. It was demonstrated that the optical activity is of negligible significance in the Raman backscattering geometry of $Bi_{12}SiO_{20}$. We interpret the peculiarities of the experimental vibrational spectrum of $Bi_{12}SiO_{20}$ based on the results of *ab initio* lattice dynamics simulations. Polarized Raman spectra were also calculated for all experimental geometries. The calculated phonon mode frequencies and polarized Raman spectra are in good agreement with the corresponding experimental data obtained in this work.

Methylammonium formate or a mixture of methylamine and formic acid: A challenge for classical molecular dynamics simulation

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Ionic polymer-metal composites (IPMCs) are hybrid materials that combine the flexibility of polymers with the conductivity of ionic media and metal nanophases. They are used in sensors, actuators, and fuel cells, where the electrolyte provides the transfer of ions between electrodes during the electrochemical conversion of chemical energy into electrical energy. Due to the shortcomings of traditional electrolytes, such as Nafion (high cost, limited stability), the search for new functional media is ongoing.

Protic ionic liquids (PILs) are a subclass of ionic liquids formed by the transfer of a proton from an acid to a base. They have high thermal and electrochemical stability and are promising electrolytes for IPMCs. However, the quantitative description of their conductivity is complicated by partial ionization and complex proton transfer mechanisms (in particular, the relay type), which requires accurate modeling of intermolecular interactions.

In this work, a force field was developed for classical MD modeling of two systems: a molecular mixture of methylamine and formic acid and an ionic liquid methylammonium formate. The parameterization of intermolecular potentials was performed based on quantum-chemical calculations of geometry and electrostatic potential. The LigParGen server and the Gaussian v.16 program were used to generate respective parameters.

MD simulations were performed using the GROMACS v2025.1 software package, with averaging over three independent trajectories. By the results of the calculations the structural and dynamic properties of the system were established. The obtained results are in good agreement with the experimental data, which confirms the correctness of the model and its suitability for further studies of charge transfer and optimization of the PIR composition for IPMCs.

Flat-band Heisenberg antiferromagnet in a magnetic field

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We consider the $S = 1/2$ antiferromagnetic Heisenberg model on a frustrated kagome-lattice bilayer with strong nearest-neighbor interlayer coupling. In the case of equal intralayer and frustrated interlayer interactions, the one-magnon spectrum of the model has a flat band, allowing us to examine its low-temperature magnetothermodynamics using a mapping onto a rhombi gas on the kagome lattice. We also compare the classical lattice-gas description with finite-size numerics to illustrate the validity of this approximation. Among our main findings are i) the absence of an order-disorder phase transition and ii) the sensitivity of the specific heat at low temperatures to the shape of the system just below the saturation magnetic field, even in the thermodynamic limit.

This study was performed together with D. Yaremchuk, V. Baliha, T. Krokhmalskii, O. Derzhko, J. Schnack, and J. Richter.

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Josephson junction dynamics with nontrivial current–phase relation

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At the early stages of the superconductivity theory development, the dependence of the superconducting current on the phase difference was sinusoidal. But over time, it turned out that such a mathematical structure of the current–phase dependence is valid for the case when the dielectric layer transparency is much less than unity. After all, the analytical dependence of the current on the phase difference for a wide range of dielectric layer transparency values is significantly different from the sinusoidal one. The shape of the current dependence on the phase difference is determined not only by the dielectric layer transparency, but also by the temperature. For the temperatures not close to the critical temperature, the method of the so-called quasi-classical equations [1] is quite widely used. Whereas for the temperatures close to the critical temperature, the well-known Ginzburg–Landau theory should be taken into account. In the current research, we consider the dynamic properties of a Josephson junction with a nontrivial current–phase relation arising in the framework of the Ginzburg–Landau theory. Namely, we consider the presence of unpaired electrons in the junction and present a separable first order differential equation describing the nonstationary Josephson effect. Despite the fact that the time dependence of the phase difference can be represented only implicitly, it made it possible to obtain an analytical formula for the oscillation period of the voltage drop. In addition to the obtained results, a more general case, which takes into account the presence of thermal fluctuations, is also considered. This research can be useful in solving a wide class of more complex problems in the theory of superconductivity.

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Generation of spin interactions using laser radiation

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A system of spins in an external single-mode coherent electromagnetic field, such as that generated by a laser, is considered. The magnetic component of the radiation affects the spin system in two distinct ways. On one hand, it leads to decoherence of the spin states. On the other hand, it induces an effective interaction between the spins. This work investigates how the parameters of the radiation influence the strength of the spin-spin interaction and, consequently, the entanglement within the system. As a practical example, the generation of interaction between the nuclear spins of phosphorus atoms embedded in a silicon matrix is analyzed.

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Abstracts

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Magnetoelectric effect in a spin-1/2 XX sawtooth chain with three-spin interactions: Exact results

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A spin-1/2 XX sawtooth chain with three-spin interactions is considered rigorously. The magnetoelectric coupling is described within the Katsura–Nagaosa–Balatsky mechanism. Using the Jordan–Wigner transformation, the Hamiltonian is reduced to a free-fermion form, and can be solved exactly. We analyze the ground-state phase diagram of the model and zero- and finite-temperature magnetoelectric effects. It is shown that quantum phase transitions can be both of the second and of the first order. At different values of the model parameters dependencies of thermodynamic functions on temperature and both fields (magnetic and electric) are obtained as well as magnetocaloric and electrocaloric effects are studied. Special attention is paid to such sets of parameters at which different quantum phase transitions occur.

Structural and collective dynamics in liquid Li along the 600 K isotherm: An *ab initio* molecular dynamics study

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A recent study of liquid Li using multi-angle energy-dispersive X-ray diffraction demonstrated a non-uniform change in structural characteristics with increasing pressure from 7.5 to 8.7 GPa along the 600 K isotherm [1]. The observed structural transformation in liquid Li under pressure correlates with the structural change in crystalline Li (the bcc-to-fcc phase transition occurring near 9 GPa). Similar behavior was previously observed in studies of liquid Pb along the melting line using *ab initio* simulations [2]. Moreover, it was found that the characteristic frequencies of transverse collective dynamics exhibit a linear dependence on increasing system density.

This work presents the results of a study of liquid Li in the pressure range of 2.0–11.0 GPa along the 600 K isotherm using *ab initio* molecular dynamics. A system of 300 particles was simulated within the density functional theory at six thermodynamic points. The calculated static structure factors show good agreement with experimental data. The analysis of the pressure-dependent coordination number distribution revealed a possible rearrangement of the local structure in liquid Li as pressure increases from 6.5 to 8.0 GPa. A two-peak structure of of transverse current correlation functions was found at high wave numbers for all pressures, corresponding to the presence of two branches in the dispersion curves of transverse collective modes. The characteristic frequencies of these branches exhibit a linear dependence on system density. Moreover, the slope of this dependence matches that observed for other monovalent and polyvalent liquid metals.

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Specific heat probes of quantum 3D Heisenberg magnets

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We consider the spin-1/2 ferro- and antiferromagnetic Heisenberg model ($|J| = 1$) on several three-dimensional lattices, that is, the simple-cubic and the diamond ones (bipartite lattices) and the pyrochlore and the hyperkagome ones (frustrated lattices), and calculate the specific heat $c(T)$ in a wide temperature range using *i)* quantum Monte Carlo simulations and *ii)* high-temperature expansion series augmented by the entropy method. The lattice geometry is important for both sings of the exchange interaction. Thus, the Curie temperature is $0.839(1)$, 0.718, $0.444\,47(5)$, and 0.330 ± 0.004 for the simple-cubic-, pyrochlore-, diamond-, and hyperkagome-lattice cases, respectively. The antiferromagnet on the simple-cubic and diamond lattices has the Néel temperature $0.946(1)$ and $0.527\,82(5)$, respectively, but does not show any magnetic order until zero temperature on the pyrochlore and hyperkagome lattices. Moreover, the specific heat obeys two sum rules,

$$e_0 = -\int_0^\infty \mathrm{d}T c(T) \quad \text{and} \quad \ln 2 = \int_0^\infty \mathrm{d}T \frac{c(T)}{T},$$

and hence contains information about the ground-state energy e_0 and low-lying excitations. Finally, $c(T)$ for the frustrated models exhibits two distinct temperature scales and the entropy associated with the low-temperature peak of $c(T)$ should match the entropy of the ground states of the Ising model on the same lattice [1,2].

This project is funded by the National Research Foundation of Ukraine (2023.03/0063, Frustrated quantum magnets under various external conditions).

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Simple model of magnetoelectric crystal. Dynamic properties

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Electric-field control of magnetic properties is possible in magnetoelectric materials, which attract a lot of interest nowadays. There are several microscopic mechanisms that drive magnetoelectricity in Mott insulators, and the so-called Katsura–Nagaosa–Balatsky (KNB) mechanism is among them. In our study, we consider a spin-$\frac{1}{2}$ chain running along the x axis, which is governed by the Hamiltonian

$$H = \sum_j \left[J \left(s_j^x s_{j+1}^x + s_j^y s_{j+1}^y \right) + J' \left(s_j^x s_{j+1}^z s_{j+2}^y - s_j^y s_{j+1}^z s_{j+2}^x \right) \right] - h \sum_j s_j^z - E \sum_j \left(s_j^x s_{j+1}^y - s_j^y s_{j+1}^x \right),$$

where J and J' stand for the isotropic XY and three-site interactions, whereas h and E for the magnetic and electric fields directed along z and y axis, respectively. The chosen geometry is important for exact solutions within the framework of the Jordan–Wigner fermionization approach. On the other hand, this system provides a simple model of a magnetoelectric with KNB mechanism [1]. We are interested in the dynamical linear response of the considered system. Following Ref. [2], we can calculate various time-dependent correlation functions related to the spin $\mathbf{s}_j$ or polarization $[\mathbf{e}_{j,j+1} \times [\mathbf{s}_j \times \mathbf{s}_{j+1}]]$, $\mathbf{e}_{j,j+1} = (1,0,0)$, which yield the quantities accessible in dynamical experiments for magnetoelectrics. With our findings, we may follow, e.g., how the electric field influences the electron spin resonance spectra.

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Active matter: From simulations of agent-based swarms to collective phases

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Active matter refers to systems of self-propelled particles that utilize internal energy stores or extract energy from the environment to generate directed motion. Due to activity, they can form the variety of spatially-ordered structures and present complex behaviors. In our work, we develop two models of such behaviors using local interaction rules with artificial fields. Agent-based simulations and molecular dynamics approach were used. In the first framework, named generalized Viczek model, we obtained mono- and polycrystallic structures. The size and orientational order of polycrystallic domains vanish with the increase of stochastic parameter. In the second framework, we added velocity- and orientation-dependent active force to the passive system, and achieved variety of phases: flocking, jamming, active crystals and active gas. The phases are characterized by orientational order parameter and mean squared displacement. Developed models demonstrate that complex behavior emerge from simple rules and can be effectively controlled by tuning a few parameters.

Triple point in a cell model with Curie–Weiss-type interaction

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We investigate a cell model of a many-particle system with Curie–Weiss-type interaction potential. It is considered as an open system in a fixed volume partitioned into a large number of congruent cubic cells. The interaction potential comprises two competing components: a global uniform attraction acting between all particle pairs in the volume and a short-range repulsion between particles occupying the same cell. Previous studies [1,2] have established that this model admits an exact solution, exhibits multiple critical points, and undergoes a sequence of first-order phase transitions. Despite variations in the interaction strengths, no triple point appears as long as these parameters remain fixed [3].

Our work is based on an analytical calculation in the framework of the grand canonical ensemble. We demonstrate that incorporating temperature-dependent attractive interactions (which is quite plausible from the physical point of view) fundamentally alters the phase behavior of the cell model. This modification preserves the model's exact solvability while resulting in the emergence of a triple point in the phase diagram.

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Influence of microscopic parameters on phase behavior of a cell model with Curie–Weiss interaction

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We investigate how varying two microscopic parameters — the cell volume, v, and the ratio between repulsion and attraction intensities, f — affect the phase behavior of a cell model with Curie–Weiss-type interaction [1]. The analysis is based on an exact solution previously derived for this model in the grand canonical ensemble [2]. At sufficiently low temperatures, the cell model exhibits multiple first-order phase transitions. By varying the cell volume and the repulsion-to-attraction ratio, we represent a quantitative comparison of the chemical potential and pressure isotherms, along with the pressure–temperature and temperature–density phase diagrams. Our results demonstrate that altering these microscopic parameters induces quantitative changes in the phase diagrams of the cell model. In particular, varying the cell volume, v, does not affect the pressure–temperature–density phase diagrams. In contrast, increasing the ratio of repulsive to attractive interaction intensities between particles, f, influences the phase diagrams by expanding the pressure range over which stable phases exist or by decreasing the critical temperature until it saturates, resulting in equal critical temperatures for all phase transitions in the sequence.

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Kinetic evolution of an open system of hard spheres with initial correlations

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The problem of the description of the kinetic evolution of a many-particle system composed of a tracer hard sphere and an environment of finitely many hard spheres in the presence of initial correlations is considered. Such initial correlations characterize systems, for example, in condensed states. We prove that the evolution of a state of a tracer hard sphere is described within the framework of the generalized Fokker–Planck type kinetic equation with initial correlations. Using an infinite sequence of explicitly defined functionals from the solution of the constructed kinetic equation, the processes of propagation of initial correlations and the emergence of correlations in the process of evolution are described.

It should be noted that in [1], the kinetic evolution of observables for such an open system of hard spheres was studied.

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Conformational transitions in stimuli responsive copolymer bottlebrushes: A dynamics study

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Stimuli-responsive polymers present an intriguing field of research due to their wide range of possible applications, and among these macromolecules are bottlebrushes with different types of side chains [1]. Developments in synthesis techniques allow chemists to create finely tuned macromolecular architectures [2]. As a result, in recent years, a number of different bottlebrushes with different types of side chains have been created. Those structures are particularly interesting, as under the influence of stimuli, they undergo a reversible conformational transition from a worm-like to a coil-like state. In addition, a collapse of this type was observed before recent developments produced macromolecules that do not clump together to form aggregates [1]. This makes them interesting for a number of applications.

In this work, we study conformational transitions for a bottlebrush with two chains grafted to each bead of the backbone with two different types of side chains grafted in alternating order. The modeling is done in three-dimensional space using a bead-spring coarse-grained model.

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Critical behavior and partition function zeros in decorated hierarchical lattices based on a triangle

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We study a class of hierarchical random graphs constructed recursively from a triangular motif, in line with the framework introduced in [2]. The graphs are built such that the motif appears at every level of the hierarchy, and randomness is introduced with random "decorations" — additional bonds connect pairs of nodes which are otherwise unconnected. Based on the strength and probability of such bonds, the system may remain ordered or disordered at all temperatures, or exhibit a nontrivial critical point. We use the exact recursive expressions for the partition function of the Ising model on a class of such graphs. These expressions are used to derive explicit expressions for the thermodynamic functions and to analyze the critical behavior of the system. In particular, we study the distribution of the partition function zeros in the complex plane, including both Lee–Yang and Fisher zeros. The latter provide tools in analysis of phase transitions and their quantitative description. The aim of this work is to clarify the nature of phase transitions and to look on the impact of the hierarchical structure on critical phenomena in these models.

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Trimer–dimer transition in one-dimensional three-component fermions with three-body interaction

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We investigate the few-body physics of a one-dimensional system composed of two impurities immersed in a sea of non-interacting fermions, interacting via a zero-range three-body force. Our focus is the competition between trimer and dimer formation, driven exclusively by the three-body interaction. Using a mixed-representation formalism, we derive an effective Hamiltonian that captures the dynamics of the impurity center-of-mass motion and its coupling to host fermions. This simplification allows for a variational treatment of this problem incorporating single particle–hole excitations both for dimer and trimer states.

Our analysis reveals that, although trimer formation is possible, the dimer state is always energetically favorable for equal masses of impurity and host fermions. The trimer state, including one extra fermion bound with the two impurities, becomes energetically suppressed compared to the simpler dimer state with particle–hole dressing. This behavior holds across a wide range of mass ratios between the impurities and the background fermions.

The resulting dimer–trimer transition line in parameter space is derived, and its physical implications for quasi-one-dimensional cold atom systems are discussed. Our findings highlight the role of many-body effects in determining the stability and composition of few-body bound states in systems with non-trivial few-body interactions.

Modeling phase separation and percolation behavior in protein-regulator mixtures under crowding conditions

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We propose a minimal coarse-grained model for a binary protein-regulator mixture under crowding conditions that is represented by a binary system of bi-functional (linkers) and tetra-functional patchy particles in a random porous medium. The porous medium is represented by a matrix of quenched at equilibrium hard sphere obstacles mimicking the crowded environment. Only heterotypic interactions between the protein and the regulatory component are considered. Critical binodals, percolation threshold lines, and fractions of free and fully bonded particles of the model at hand are calculated in the framework of extension and combination of Wertheim's thermodynamic perturbation theory for associating fluids, the scaled particle theory, and the Flory–Stockmayer theory for chemical gelation. In agreement with previous experimental findings, we have shown that increasing the interaction strength (affinity) between linkers and particles at fixed temperatures extends the phase coexistence region, and as a consequence increases the critical temperature and slightly decreases the critical density of the mixture. On the other hand, we found a significant narrowing of the phase coexistence region, both critical density and temperature decreasing, and extending the percolating phase at the obstacle packing fraction increasing. Thus, changing the packing fraction of the porous medium, which acts as an external field, we predict how the intracellular environment may affect the phase separation, percolation properties, and protein interactions of the model mimicking associating protein-regulator mixtures within cells.

The recoherence/decoherence processes in a single qubit dephasing model

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We study the recoherence/decoherence events in the simple spin-boson dephasing model [1]. The open quantum system [2] is prepared in the initial state obtained by a special kind of the non-selective measurement. At such a measurement, the correlational contribution to the generalized decoherence function [3–4] does not depend on the qubit parameters and ensures the coherence enhancement at the initial staged of the system evolution, if the coupling strength is large enough.

The recoherence times t^* and the maximum values of the recoherence increments γ_{extr} are studied as the functions of coupling strengths λ, ohmicity indexes s and temperature T. We found that the sub-Ohmic and Ohmic regimes are more favourable for the recoherence than the super-Ohmic one. The most interesting observation is that the short time behaviour (when the recoherence takes place) and the long time dynamics (the decoherence at large t) can be closely related: the domain of s, where the decoherence changes its type (from the complete to incomplete one [1]) is, simultaneously, that of the weakest recoherence. The obtained results give us some hints about the basic characteristics of the bath, which can provide the most optimal values of t^* and γ_{extr} in some sense.

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Ising model in the Rényi statistics: The finite size effects

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The basic principles of the Rényi statistics [1] are applied to describe the finite-size effects in the 1D Ising model. Unlike the traditional approaches [2–3], when the subsystem is placed in the predefined environment of fixed size, we consider a part of the system under study itself to be a reservoir.

The internal energy and temperature of the subsystem are derived using the Rényi distribution and are assumed to be equal to the analogous quantities obtained in the microcanonical ensemble. This allows us to calculate self-consistently the Rényi index q and the Lagrangian parameter T, to relate them to the physically observed temperature $T_{\rm ph}$, and to show that the entropic phase transitions are possible over a wide range of temperatures [4]. It is shown that the parameters q and T have a jump with increase of the subsystem size L, after which the Rényi entropy S_R becomes a slightly non-additive function of L. At the same time, there are no temperature phase transitions in the system.

We have verified numerically that the relation $q \approx 1 + k_B/C_{VE}$ is satisfied in the whole region of L to the left of the entropic phase transition point, where C_{VE} denotes the heat capacity of the reservoir. To the right of the transition point, in a narrow region of L, another relation $q \approx 1 - k_B/C_{VE}$ is valid [1]. At the transition point, the well-known limit $\lim_{\eta\to 0} \partial S_R/\partial\eta = 1/2C_V$ is satisfied, where $\eta = 1 - q$ plays the role of an "order parameter" and C_V denotes the heat capacity of the subsystem. Summarizing, unlike the traditional approaches [1–3], we can describe the subsystem behaviour in the entire range of the Rényi indexes: from $q \to 1$, which corresponds to the canonical Gibbs distribution, to $q \to 0$, which corresponds to the microcanonical distribution.

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Interaction of colloidal particulates with microstructured thermo responsive polymer brush: computer simulations

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Microstructured surfaces composed of adherent domains and stimuli-responsive polymer domains (that undergo swelling-shrinking upon temperature change around the low critical solution temperature, LCST) were proven to catch and release colloidal particulates (CP) effectively [1]. Contrary to the uniform stimuli-responsive structures, their micropatterned counterparts allow decoupling and fine tuning the properties of their sticky and push-off regions in a broad range. We consider the adsorption and desorption of particulates on the stimuli-responsive surface made of tethered polyacrylic acid (PAA) domains that contain the adherent functional motifs and thermoresponsive poly(N-isopropylacrylamide) (PNIPAM) domains, both arranged into regular micropatterns. At temperatures above PNIPAM LCST, the PNIPAM domains collapse in water, allowing the adsorption of the particulates on the PAA regions. When cooled below LCST, PNIPAM swells and pushes particles off the surface. We develop coarse-grained models for all the components for particles on the microstructured surfaces and use computer simulations to analyze the optimal structure in terms of the PAA chain length, types of the micropatterns, the ratio between surface areas of the PAA and PNIPAM domains, and micropattern graininess in relation to particle dimensions [2]. The study is relevant and motivated by the problems of harvesting and sorting prokaryotic and eukaryotic cells on microstructured surfaces. Supported by NAS/ONRG grant 7115, NSF grant 2401713, computing time by NRFU grant 2023.05/0019.

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Statistics of the self-affine regime of traffic flow

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Traffic flows are stochastic systems with complex internal dynamics that depend on both internal and external fluctuations. In this work, we investigate the dynamics of traffic flow based on a stochastic model constructed from the Fokker–Planck equation. The model accounts for both the flow density and velocity, as well as the influence of noise modeling random disturbances.

Using the Fokker–Planck equation, we analyze the stationary probability distributions. It is shown that under certain conditions, the system exhibits self-similar behavior. This regime is characterized by a power-law distribution of probability density and indicates the presence of long-term correlations and the absence of a characteristic scale.

Numerical simulations performed using the Euler method confirmed the analytical predictions. In the case where the noise intensity acting on velocity significantly exceeds the noise in vehicle density, the system demonstrates scale-invariant fluctuations typical of self-organized states.

The obtained results provide deeper insight into the mechanisms of traffic jam formation and irregular transitions between traffic regimes. This is important for developing more accurate models for predicting traffic dynamics and optimizing road infrastructure.

How different head groups affect binding of passivating ligands to $CsPbBr_3$ nanocrystals: Insights from atomistic simulations

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$CsPbX_3$ (X = Cl, Br, I) cesium lead halide perovskite nanocrystals (NC) have emerged as leading materials in the field of optoelectronics due to their exceptional properties, such as narrow emission bandwidths, high photoluminescence quantum yields, and tunable emission wavelengths. Their compatibility with low-temperature, solution-based processing further enhances their suitability for use in next-generation technologies, such as light-emitting diodes, displays and quantum emitters. To ensure the long-term performance of nanocrystals, surface ligands are employed during both synthesis and purification. They prevent aggregation by providing steric or electrostatic repulsion, and they modulate the reactivity and structural integrity of the NCs.

In this study, we examine how different ligand head groups, such as carboxylate, phosphate, and sulfate, affect binding of passivating ligands to $CsPbBr_3$ nanocrystals. For each system, we perform all-atom MD simulations in slab geometry with an explicit solvent environment. The solvent is represented as a 1:1 mixture of toluene and acetone, which is the medium typically encountered during NC purification. The free energy profiles are calculated via umbrella sampling method. The ligands binding free energies are extracted and compared.

Diffusion of hard-sphere mixture in disordered porous media from a new extended Enskog theory

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A new extended version of Enskog theory (NEET) was proposed recently [1] for the description of the self-diffusion coefficient of hard-sphere fluid adsorbed in a matrix of disordered hard-sphere obstacles. In this report, the NEET approach is generalized for the description of the diffusion of hard-sphere mixtures in porous media. As the input information for this theory, we take into account that the fluid particles can be either hindered in their motion by cages formed by other mobile fluid particles or trapped by the immobile matrix particles. We show that complex dynamics of fluid mixture in random porous media strongly correlates with the ratio of thermodynamic porosities of each species and the total thermodynamical porosity to geometrical porosity previously introduced by us for the description of thermodynamical properties of hard-sphere fluid in random porous media. These ratios are interpreted as the fractions of volume-free matrix particles and of fluid particles trapped by matrix particles. The comparison of the obtained theoretical predictions results with computer simulations data [2] for a binary hard-sphere mixture in random hard-sphere porous media is presented.

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Modeling displacements of near-surface ionic layers in semi-infinite metallic systems

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For the model of a semi-infinite metal with a flat metal–vacuum separation surface proposed in [1], the effective Hamiltonian of the ionic subsystem is obtained by averaging over the subsystem of electrons in the adiabatic approximation [2]. The interaction of ions with a negatively charged electron layer located outside the metal leads to displacement $\vec{\xi}_n$ of the ionic layers relative to their positions $\vec{R}_n^0$ in the metal without a separation surface ($\vec{\xi}_n = \vec{R}_n - \vec{R}_n^0$). These displacements must minimize the free energy F of the semi-infinite metal, i.e. satisfy the condition

$$\mathrm{grad}_{\vec{\xi}_n} F = 0.$$

In the quadratic approximation by $\vec{\xi}_n$, an expression for F is obtained, from which the equation for finding $\vec{\xi}_n$ is derived.

We show that in the absence of a near-surface electron layer with density $n(\vec{r})$ ($n(\vec{r}) \equiv 0$), the equation for $\vec{\xi}_n$ has only a trivial solution.

For $n(\vec{r}) \neq 0$, a numerical solution of the aforementioned equation is found and it is shown that $1 \div 2$ near-surface ionic layers are subject to displacement, for which $|\vec{\xi}_n| = (0.03 \div 0.16)d$, where d is the lattice period of the metal when the surface is absent.

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From Zeros to Exponents: Critical and tricritical behavior in the Blume–Capel model on a complete graph

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The behavior of the three-state Blume–Capel spin model (spins take values ±1 and 0) on a complete graph was analyzed for the first time using the formalism of partition function zeros [1]. On a complete graph, all spins interact with equal strength — equivalent to the mean-field approximation, so in the thermodynamic limit the problem is exactly solvable. However, the onset of a phase transition on finite-size graphs have been less explored. Finite-size scaling (FSS) is an effective method for studying critical behavior in finite systems. The partition function zeros method provides an alternative approach: by analyzing universal ratios and asymptotic properties of the partition function zeros in a complex plane, one can determine the critical exponents governing a phase transition. It was demonstrated that FSS analysis via partition function zeros allows studies of much smaller systems than standard thermodynamic quantities while achieving the same accuracy in critical exponent estimates. This efficiency is important for conserving computational resources in simulations. The zeros of the partition function were investigated in the complex temperature plane (Fisher zeros), in the complex external magnetic field plane (Lee–Yang zeros), and in the complex crystal field plane. Differences between critical and tricritical behavior were studied, with a focus on the crossover between these regimes in finite-size systems.

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Adsorption of disk-like particles on a patterned adhesive surface

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We investigate the adsorption behaviour of disk-like particles on a patterned attractive surface represented by an ordered array of circular adhesive domains. Our aim is to clarify how the size of these domains affects the adsorption isotherms of the particles. To this end, we consider a two-dimensional model of hard-disk particles interacting with the domains via an attractive potential proportional to the overlap area between a disk particle and the adhesive regions. Using Monte Carlo simulations in the grand canonical ensemble, we obtain adsorption isotherms describing the particle density as a function of the chemical potential. Our results show that the adsorption behaviour is highly sensitive to the size of the adhesive domains, not only quantitatively but also qualitatively, leading to additional inflection points on the isotherms. We also find that the adsorption efficiency does not scale monotonically with domain size and can vary significantly depending on the chemical potential. In particular, when the particle and domain sizes are equal, the adsorption efficiency reaches a maximum at intermediate values of the chemical potential, but this efficiency decreases as the chemical potential increases further. These findings contribute to the understanding and prediction of adsorption phenomena on nano- and micro-structured surfaces.

Some liquid–gas equilibrium regularities in view of global isomorphism approach

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Liquid–gas equilibrium is considered using the global isomorphism with the Ising-like (lattice gas) model. Such an approach assumes the existence of the order parameter in terms of which the symmetry of binodal is restored not only in the vicinity of the critical point (critical isomorphism) but globally in whole coexistence region. We show how the empirical law of the rectilinear density diameter of the liquid–gas binodal allows to derive rather simple form of the isomorphism transformation between fluid and lattice gas model of Ising-type:

$$\rho = \rho_* \frac{x}{1 + z\tilde{t}}, \quad T = T_* \frac{z\tilde{t}}{1 + z\tilde{t}}.$$

Here $x = \langle n_i \rangle$ is the lattice gas density, $\tilde{t} = t/t_c$ is the temperature t normalized to the critical one t_c. The relations for critical parameters which follow from such isomorphism are tested on a variety of fluid systems both real and model ones. Its parameters T_*, ρ_* appear to be sensitive to the liquid binodal instability known in hard-core Yukawa attractive fluids (HCAYF). Also we consider the phase equilibrium in polymer solutions and the Flory θ-point as the extreme state of such equilibrium within our approach. The most crucial testing is in $2D$ case using the Onsager exact solution of the Ising model and we represent the results of our approach to the calculation of critical point parameters of monolayers for noble gases and the surface tension. We also discuss the microscopic nature of such a correspondence between continuous fluid and lattice model basing on the distribution of values of pair interaction $\Phi(r_{ij})$ potential.

Application of the zero-range potential model for calculation of electronic structure of molecules

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We calculate the energy spectra and the ionization energies of molecules using the zero-range potential (ZRP) model. The ionization energies of separate atoms and the lengths of electron bounds are the only input parameters. Within the ZRP method, the problem of finding a wavefunction of a bound state is reduced to a purely algebraic problem of finding non-trivial solutions of linear algebraic equation systems. This way the electronic structures of diatomic molecules such as hydrogen and lithium hydride, as well as molecules with high symmetry such as methane and ammonia, and molecules of stable compounds C_{20} are considered in a unified manner. The only difference is the amount of calculations needed for evaluating the energy spectra of molecules as it grows when the number of atoms in a molecule increases. But for molecules of high symmetry, it is possible to simplify the calculations as was demonstrated in the cases of methane, ammonia, and stable compounds of C_{20}. The results are very close to the experimental data with deviations less than 5%. With such simplicity and precision, the ZRP method can be considered as an alternative to the density functional and ab initio methods. Further development of the ZRP model to incorporate individual characteristics of composite systems results in getting a simple tool to describe the electronic properties not only of single molecules but also quantum dots and low-dimensional localized defects.

Features of kinetics in a two-level system with time-dependent coupling to a boson field

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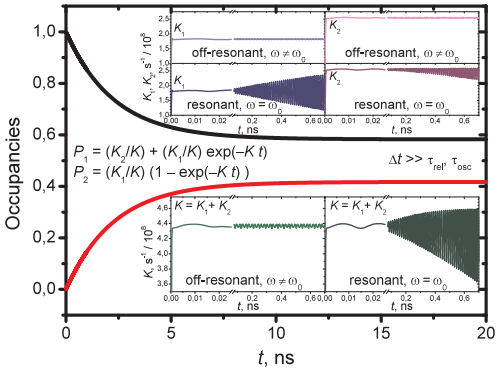
The interaction of a dynamic system with the environment plays a key role in kinetic processes responsible for establishing the probabilities of the system being in a stationary or quasi-stationary state. If the interaction with the environment is large compared to the interaction leading to transitions between states of the dynamic system, then polaron-like states are formed. In the harmonic approximation, each of them is considered as a state dressed in a "phonon coat". It is formed due to the coupling of the states of the dynamic system with the phonons of the environment (the boson field).

We have investigated a special regime of formation of polaron-like states, when the coupling of the system with the optical vibrational mode depends on time, and the remaining modes of the environment belong to the phonon (boson) bath. Following the approach developed in the work (ref. doi: 10.15407/ujpe69.8.552), the kinetic processes in a two-level system (TLS) were investigated. A number of features have been found that are caused by the periodic time dependence of the coupling between TLS states and the optical vibrational mode. The example is the resonant behavior of the transition rates K_1, K_2 and $K = K_1 + K_2$ (see figure). It is shown that the resonant is observed when the frequency ω of oscillations of the parameter characterizing the coupling of the TLS with the optical mode coincides with the frequency ω_0 of the mode. As for the probabilities of states P_1 and P_2, due to the "coating" their behavior over time is smoothed out.



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Numerical simulations to characterise phase transitions in the loss landscape of neural networks with L2 regularisers

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Neural networks are commonly trained by tuning their parameters, weights and biases of each neuron, such that a loss function is locally minimised. Even in a local minimum the model can overfit, reducing its capability to recognise patterns in unseen data. Often L2-regularisers are used to avoid overfitting. However, small changes in the regularisation strength ($\approx 10^{-11}$) can lead to drastic changes in model accuracy. Here we show this effect explicitly for neural networks trained on the MNIST data set. The observed drastic changes in accuracy correspond to first-order phase transitions in the parameter and loss spaces. We analyse the vicinity of those phase transitions by extensive numerical simulations, calculating refined time-resolved curvature and distance measures related to the loss landscape, in particular eigenvalues and eigenstates of the Hessian. We, thus, provide a thorough analysis of the role played by the error landscape itself and of the additional effects due to regularisation. Our results lead us to propose a new numerical framework to obtain information in those transition regions that would otherwise be inaccessible in the standard framework. Our aim is to connect these phase transitions with the curvature of the loss landscape, without regularisation, and categorise the different phase transitions that appear.

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

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The exactly solvable spin-1/2 distorted diamond Ising–Heisenberg chain which contains ferromagnetic Ising interaction and antiferromagnetic *XXZ* Heisenberg interaction in the presence of the external magnetic field is investigated. This chain exhibits a geometric frustration of spins. The influence of quantum fluctuations, the distortion, and the magnetic field on the ground state, magnetic and thermal properties of the model are studied in detail. In particular, it is established that the zero-temperature magnetization curve may involve intermediate plateaus at zero and one-third of the saturation magnetization. It is demonstrated that the temperature dependence of the specific heat shows up to three distinct peaks at zero magnetic field. The physical origin of all observed additional peaks of the specific heat was clarified on the grounds of dominating thermal excitations.

Mixed spin-(1,1/2) Ising–Heisenberg distorted diamond chain with ferromagnetic Ising and antiferromagnetic Heisenberg interactions

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Ground state and thermodynamical properties of the exactly solvable mixed spin-(1,1/2) Ising–Heisenberg distorted diamond chain in the presence of the external magnetic field is rigorously studied in the frustrated case of ferromagnetic Ising and antiferromagnetic *XXZ* Heisenberg interactions. The influence of quantum fluctuations, the distortion, and the magnetic field on the ground state, magnetic and thermal properties of the model are studied in detail. In particular, it is established that the zero-temperature magnetization curve may involve intermediate plateaus at zero and one-half of the saturation magnetization. It is demonstrated that the temperature dependence of the specific heat shows up to three distinct peaks at zero magnetic field. The physical origin of all observed additional peaks of the specific heat was clarified on the grounds of dominating thermal excitations.

Two-phase structure in the Bose–Einstein condensate dark matter model

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To accurately describe astrophysical observables in models of self-gravitating Bose–Einstein condensate dark matter (BEC DM), it is essential to incorporate the self-interaction (SI) among ultralight bosons. In particular, simultaneously including two- and three-particle SIs gives rise to novel phenomena—a two-phase structure and an associated quantum first-order phase transition at zero temperature [1,2]. Replacing the polynomial SI with an axionlike periodic potential not only reproduces these results via non-perturbative solutions of the stationary Gross–Pitaevskii equation [3] but also complicates the phase diagram by the appearance of additional, including unstable, phases and transitions [4]. The axionlike SI can be also involved in the formation of composites—specifically, dimers—from DM particles [3].

Applying this framework to DM-dominated dwarf galaxies, such as NGC 2366, reveals a first-order phase transition (PT1) driven by quantum fluctuations in particle density. This transition marks an abrupt shift from a diffuse state to a denser configuration, even though the DM parameters of NGC 2366 suggest a continuous, supercritical behavior. Notably, PT1 also serves as a thermodynamic indicator that distinguishes between stable and unstable configurations. When a dense phase nucleus (core) forms—reaching a threshold of about 12% of the total mass—the enhanced gravitation provides stability against fluctuations. In comparison, the dense DM of NGC 2366 comprises roughly 19% of the mass while occupying only 4.7% of its total volume [4].

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Microscopic structure and energetics of Li+ ion solvation in benzonitrile: MD simulations vs. quantum chemistry calculations

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Modern approaches to the design of electric energy storage devices based on electrochemical double-layer capacitors (supercapacitors) and their hybrids with Li-ion batteries are currently considered as one of the alternative ways to develop a new generation of electrochemical devices. For such hybrid devices, it is desirable to use solutions of chemically stable lithium salts in acetonitrile (AN) as electrolyte, which are common in lithium-ion battery technology [1]. However, the correspondingly low boiling point of AN prompts the search for alternative solvents. In this regard, benzonitrile (BN) can be considered as a high-temperature analog of AN with acceptable dielectric constant and viscosity values.

Herein, we report the energetics, microscopic structure and dynamics of Li-ion solvation shell in BN by using quantum chemical calculations (QCC) and molecular dynamics (MD) simulations.

The force filed (FF) for BN were generated by using the combination of OPLS-AA [2] intramolecular and short range intermolecular potentials and partial charges calculated at the M062X/6-311++G(d,p)/ChelpG level. The proposed FF of BN allows one to reproduce with satisfactory accuracy the experimental values of its enthalpy of vaporization and self-diffusion coefficient.

The microscopic structure of the investigated ion-molecular system was analyzed in terms of radial distribution functions and the running coordination numbers. The analysis of the time correlation functions allowed us to establish a significant influence of Li^+ ion on translational, rotational and reorientational dynamics of solvent molecules within the ion first solvent shell.

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The dynamics of the spinful impurity in ideal Bose gas

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We consider model describes a system of macroscopic number N of mutually non-interacting Bose atoms loaded in large volume V with periodic boundary conditions that interact, through the δ-potential, with a spin-1/2 static particle. The bosonic medium induces the effective two-body, three-body, and higher-order inter-spin interactions. However, all of them are of the Ising type. By solving the Heisenberg-like equations for bosonic creation and annihilation operators, we calculate the time evolution of the wave function or density matrix of the initially non-interacting system. Then, tracing out bosonic degrees of freedom, one obtains the reduced density matrix of spin. Two distinct situations considered: the zero-temperature evolution in the medium of bosons in the BEC state and the finite-temperature case with bosons in thermal equilibrium. We have found that both the entanglement properties and decoherence dynamics crucially depend on a sign of the boson–impurity coupling.

Magnetothermodynamics of the antiferromagnetic Heisenberg model on the Tasaki lattice in an external magnetic field

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The Tasaki lattice represents an example of a highly frustrated two-dimensional antiferromagnet. It is a decorated structure formed by placing three sublattice sites within the unit-cell of a square lattice.This geometric construction give rise to a flat magnon band and geometric frustration, making the Tasaki lattice an ideal model for exploring magnetothermodynamics properties in strongly frustrated antiferromagnets.

We study the $S = 1/2$ antiferromagnetic Heisenberg model on the Tasaki lattice in the presence of a uniform external magnetic field h. Our analysis focuses on the regime near the saturation field, specifically for $h = 0.99h_{sat}$ and $h = 1.01h_{sat}$, where $h_{sat} = 12|J|$ is the field required to fully polarize the system. Using analytical methods, we derive compact expressions for several key thermodynamic quantities as functions of temperature T and magnetic field h, including magnetization $M(h)$, magnetic susceptibility $\chi(T, h)$, specific heat $C(T)$, and entropy $S(T)$. Our approach explicitly accounts for the number of spins N in the system, allowing direct generalization to the case of an infinite lattice ($N \to \infty$).

To validate our theoretical framework, we perform exact diagonalization on the Tasaki lattice for small N. The numerically obtained magnetothermodynamic curves show excellent agreement with our analytical predictions in the low-temperature regime. This comparison confirms the accuracy and consistency of our analytical approach.

Furthermore, this comparative study highlights the pivotal role of flat-band magnon physics in governing the low-temperature magnetothermodynamic behavior near the saturation field. Our results establish a foundation for understanding magnetothermodynamic properties in frustrated, low-dimensional quantum magnets.

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Systematic investigation of density fluctuations in laser wakefield accelerators on the properties of the accelerated electrons

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Fundamental questions on the nature of matter and energy have found answers thanks to the use of particle accelerators. However, the accelerating field in superconducting radio-frequency cavities due to electrical breakdown is limited to about 100 MV/m. This limits the amount of acceleration over any given length, requiring very long accelerators to reach high energies. To overcome this limitation, novel acceleration techniques are being explored, including plasma wakefield acceleration, that can exceed an accelerating gradient of $E > 100$ GV/m.

Until now, almost all Laser Wakefield Acceleration (LWFA) simulations have assumed smooth plasma density profiles, but recent few-cycle shadowgraph imaging of the acceleration process has revealed small density fluctuations in the plasma profile. The main focus of this project is on a simulation study of the nonlinear laser-plasma interaction using the particle-in-cell code PIConGPU, and based on measured density profiles, we want to determine the difference in electron beam quality after the LWFA process caused by the non-smooth density.

Bose condensate in low-dimensional bosons with three-body interaction

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Inspired by the narrow Feshbach resonance in systems with a two-body interaction, we propose a two-channel model of three-component bosons with a three-body interaction that includes the finite-range effects in low dimensions.

Applying this effective description to the system of single-particle bosons and compound three-particle bosons (trimers), we investigated its many-particle properties. From the assumption that the interaction in the system is weak and applying the mean-field approach, we build the phase diagram.

Using the Bogoliubov approximation, we obtained two branches of the elementary excitation spectrum and calculated the Bose condensate depletion for single particles and trimers. The latter allowed us to analyze the applicability limits of the approximated second quantization method to the problem.

Binodal and its diameter for Morse fluids near the critical point

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The present work has focused on the investigation of Morse fluid behavior near the critical point within the framework of a cell model. The vicinity of the critical point is of both fundamental and practical interest, while also being challenging to analyze due to the significant role of fluctuation effects.

An analytical procedure has been developed for constructing the liquid-gas coexistence curve and calculating its diameter in the critical region. The numerical evaluation of the relevant quantities has been illustrated using Morse potential parameters typical for sodium. The critical point parameters for liquid alkali metals, sodium and potassium, previously obtained within our approach, are consistent with available experimental data.

The analysis of the relationship between density and chemical potential at subcritical temperatures has enabled the derivation of equations describing the liquid-gas coexistence curve in the temperature-density plane. An explicit expression has been derived for the analytical temperature-dependent term appearing in the equation for the rectilinear diameter of the binodal. The upper part of the liquid-gas coexistence curve and its diameter have been constructed both with and without including the analytical temperature-dependent term in the calculation. A condition has been established that improves the agreement of the presented binodal branches with Monte Carlo simulation data from other study, extrapolated to the immediate vicinity of the critical point. It has been clearly demonstrated that better agreement is achieved when the analytical temperature-dependent term is neglected in the calculation of the gas branch, but retained in the calculation of the liquid branch.

The analytical approach developed for a simple fluid system may prove useful for investigating the critical behavior of multicomponent fluids. The present study also represents a certain methodological contribution to the theoretical description of critical phenomena.

Entropy of a multiple-occupancy cell fluid model

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We consider a statistical cell fluid model with unrestricted cell occupancy and infinite-range (Curie–Weiss) interactions. Each cell can host arbitrarily many particles, all pairs experience a uniform mean-field attraction, and a local repulsive interaction stabilizes the system. In the thermodynamic limit, the model is exactly solvable and exhibits a hierarchy of critical points analogous to a generalized Curie–Weiss magnet. We derive an analytical closed-form expression for the entropy in this model. This allows us to examine the entropy's behavior in detail near the multiple critical points and in different phases.

Notably, at sufficiently low temperatures the reduced entropy per particle S^* versus density shows cusp-like minima at around whole-number reduced densities $\rho^* \approx 1.0,\ 2.0,\ 3.0,\ \ldots$ (here, ρ^* is the average number of particles per cell). For example, as ρ^* approaches 1, S^* drops to a minimum (indicating a loss of configurational freedom) and then rises again once ρ^* exceeds 1. We discuss an explicit parallel with the analogous entropy cusps in the Hubbard model (De Leo et al., Phys. Rev. A **83**, 023606 (2011)).

This work underlines the rich thermodynamics of multi-occupancy cell models and the utility of exact entropy formulations for uncovering subtle system features.

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Modeling of distributions of the magnetic flux in long Josephson junctions with nontrivial current-phase relation

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In numerous studies (see review [1]) dedicated to the study of superconducting tunnel junctions, the electron transmission coefficient is considered small, which results in small current values. When studying the current–phase relationship without additional conditions on the electron transmission coefficient, it is necessary to consider depairing effects. Since the transparency coefficient varies over a wide range of values, the current magnitude can reach values close to the thermodynamic critical value. Due to significant current values, the so-called depairing effect becomes significant. Taking this effect into account leads to a deviation of the current–phase relationship from sinusoidal [2], which will obviously also affect the magnetic properties of superconducting junctions.

The aim of this research is the investigation of the effect of the deviation of the current–phase relationship from sinusoidal on the magnetic field penetration into a superconducting junction and the evolution of fluxons. We consider the two-dimensional case, i.e., when the phase difference depends on two coordinates in the plane of the junction.

A novel two-dimensional second-order partial differential equation that describes the phase dynamics in the Josephson junction and takes into account the flow of unpaired electrons across the junction is proposed. It has the form of the two-dimensional modified sine-Gordon equation with the nontrivial current–phase relation. The spatial behavior of the penetrated magnetic flux quantum (Josephson vortex or fluxon) is analyzed for the different values of the insulating layer transparency. The proposed equation of motion is used to investigate the dependence of the equilibrium fluxon velocity on the constant bias current for the different values of the insulating layer transparency.

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Using word analysis to study single-file chain of water molecules in electric field

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Confinement of the water molecules dramatically changes their dielectric properties. It was demonstrated that the in-plane dielectric constant of a 2-dimensional system of water molecules, just a few molecules thick, reaches abnormally large values compared to bulk water [1]. One-dimensional system of water molecules was also studied experimentally [2] and it was shown that there is a quasi phase transition in such a chain. Moreover, the chain was studied using molecular dynamics and quantum chemistry approaches as well as statistical physics [3], where the authors suggested a simple lattice model. Based on the results presented in [3], we decided to add to the model one more parameter — the external electric field, to study how its presence affects properties of the molecular chain. One possible way to numerically solve this problem is to view the microstates of the chain as "words". To calculate the partition function for a given number of molecules, each "word" can be generated by the `itertools.product()` function and analyzed using the `re.findall()` function in the Python programming language.

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Interaction topology effect on collective decision-making with heterogeneous biases

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The accuracy of collective decision-making in groups is shaped by a complex combination of factors, including prior knowledge, individual biases, social influence, and the structure of the interaction network. In this study, we explore a spin model that incorporates individual biases and allows for tuning the nonlinearity of social interactions [1]. Extending earlier analyses conducted on fully connected networks [2] and regular two-dimensional lattices [1], we examine how transitioning to sparser, random network topologies influences group decision dynamics. To quantify the system's sensitivity to both internal and external perturbations, we apply two distinct measures of susceptibility. A key focus of our investigation is how the peak in susceptibility varies with changes in network connectivity. Our results suggest that collective systems may be able to maintain high responsiveness to environmental variability by adapting either their interactions or the structure of their networks to stay near the point of maximal susceptibility [3].

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Reaction–diffusion processes in structurally heterogeneous media: A Monte Carlo study

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We investigate the survival problem for mobile target-particles B in a two-dimensional medium containing mobile traps A, which can either annihilate or coagulate with each other $A + A \to (\varnothing, A)$ and react with targets as $A + B \to A$ [1–3]. The medium includes randomly placed quenched defects, which block particle motion and act as permanently inaccessible sites. Using Monte Carlo simulations, we show that the average B-particle density decreases more slowly and reaches a nonzero value in the presence of disorder, compared to the pure lattice. Since defects may trap particles in isolated regions, we focus on percolation clusters of connected empty sites that can be visited by both A and B particles. The percolation structure is identified using the Hoshen–Kopelman algorithm and verified with standard graph search methods. We calculate the fractal dimension of the clusters and study how the decay of B-particle density depends on defect concentration. Our results show that structural disorder strongly affects the dynamics of reaction–diffusion systems.

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Structure factor and dynamic structure factor of one-dimensional ion conductors

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The energy spectrum of a one-dimensional finite ionic conductor with periodic boundary conditions was calculated within the framework of the extended hard-core boson lattice model using the exact diagonalization technique. The single-particle correlation was investigated in this research, and structure and dynamic structure factors at temperature $T = 0$ were calculated. The presence of long-range single-particle correlation in the superfluid-type phase (SF) is shown. The presence of an ordered modulated (CDW) phase at the half-filled ion positions (density $\rho = 0.5$) is confirmed by the obtained maxima of the structural factor at $k = \pi/a$, and by the maxima of the dynamic structural factor in the frequencies diapason corresponding to the energy of the band gap. The presence of maxima of the dynamic structural factor $S(k, \omega)$ in the region of low frequencies at $\rho = 0.25$ confirms the possibility of the existence of a superfluid phase of an ion conductor.

Description processes of the interaction of water and aqueous solutions with fuel-containinig materials in the New Safe Confinement of the "Shelter" object

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The main mechanisms and conditions of interaction of lava-like fuel-containing materials (LFCM) with the atmosphere, water and aqueous solutions are presented [1]. The mechanisms of destruction of the LFCM surface, including ion-exchange processes, hydrolysis, dissolution, oxidation, etc., were analyzed. Inhomogeneous diffusion coefficients for UO_2^{2+}, Cs^+ ions at the interface "aqueous solution of radioactive elements — LFCM" were calculated. The interdiffusion processes and the rate of penetration into the porous medium of the reaction front of the internal hydrolysis of the silicon-oxygen network during interaction with an aqueous solution were analyzed, the reaction and adsorption processes are hidden in the rate of internal hydrolysis.

Since there is a decrease in humidity in the modern conditions of New Safe Confinement of the "Shelter" object, based on the calculations, it can be concluded that the diffusion of uranium and other transuranic atoms also decreases. And that is obviously good. However, in the processes of dust suppression in the SO with liquid mixtures of a localizing polymer coating and a liquid with gadolinium (previously it was from 45 tons to 90 tons per year), there is a problem of disposal of radioactive water, which obviously interacts in certain places with LFCM, in particular in the lower rooms. In connection with the continuous α-β-γ–irradiation of the aqueous solution from the surface of the LFCM, tracks of densely ionized plasma are constantly formed in the near-surface layer, consisting of electrons, ions H^+, OH^- are products of the decomposition of water molecules, as well as ions present in the aqueous solution Na^+, CO_3^{2-}, HCO_3^-, UO_2^{2+}, PuO_2^{2+}, Cs^+, Sr^{2+}, etc. Complex diffusion, adsorption, oxidation-reduction processes take place in this near-surface region, accompanied by the processes of hydrolysis by H^+, OH^-, Na^+, Ca^{2+} ions and polymerization of the silicon-oxygen network, leaching of ions from the surface of the LFCM.

1. M.V. Tokarchuk et al. Condens. Matter Phys. **28**(1) (2025) 11601.

To the generalized equations of hydrodynamics for viscoelastic fluids in fractional derivatives

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We present the general approach for obtaining the generalized transport equations with the fractional derivatives by using the Liouville equation with the fractional derivatives for a system of classical particles and the Zubarev nonequilibrium statistical operator method within the Gibbs statistics. In this approach, we obtain the non-Markov equations of hydrodynamic in a spatially non-homogeneous medium with a fractal structure [1]. We analyze the structure of generalized viscosity and thermal conductivity transfer coefficients, and cross transfer coefficients. In the Markov approximation (there is no memory in time) and neglecting spatial heterogeneity, the generalized equations of hydrodynamics can be reduced to equations of hydrodynamics for a continuous medium with a fractal structure.

In the case of isothermal processes we obtain a system of equations for nonequilibrium average values of particle number densities and their momentum, which can describe non-Markovian viscoelastic processes in liquids. They account for spatial fractality and memory effects in the generalized fluid viscosity. It is obvious that the spatial fractality of the system affects the processes of particle transport, and this influence, in particular, can manifest as temporal multifractality with characteristic relaxation times. In this regard, we modeled the non-Markovianity of viscoelastic processes in time, choosing the frequency dependence of the memory function, in particular in the form $[(1 + i\omega\tau)^{1-\gamma}]^{-1}$, with a characteristic relaxation time τ corresponding to the generalized Maxwell model for a viscoelastic fluid.

1. P. Kostrobij et al. Phys. Fluids **37**(7) (2025) 073118 (2025).

To the kinetic theory of dense gases and liquids. Calculation of quasi-equilibrium particle distribution functions by the method of collective variables

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Based on a chain of BBGKI equations with a modified boundary condition that takes into account multiparticle correlations, kinetic equations in the approximate "pairs" collisions and in the polarization approximation, taking into account the interaction through the third particle, obtained. The specifics of the model representation of the pair potential of particle interaction through short-range and long-range parts were taken into account. In the case of the short-range potential in the form of the potential of solid spheres, the contribution of Enskog's revised theory to the complete integration of the collision of the kinetic equation is obtained. The collision integrals include paired quasi-equilibrium distribution functions that depend on the nonequilibrium mean values of the particle number density and the inverse temperature. The method of collective variables Yukhnovskii is applied for the calculation of pair quasi-equilibrium distribution function with an allocation of short-range and long-range parts in the potential of the interaction of particles. In this case, the system with short-range interaction is considered as a frame of reference.

1. M.V. Tokarchuk, Math. Model. Comput. **9**(2) (2022) 440.

Role and place of classifications for the creation and the development of modern physics

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Main problems of role of classifications for the creation and the development of modern physics are discussed [1,2]. An example of such a classification is the theory of crystallographic groups (F.E. Neumann, A.M. Schoenflies and E. Fedorov), which allowed to link the symmetry properties of physical objects with their physical properties [2]. Later, E. Wigner extended this approach to continuous groups (Lie groups), which played an important role in the development of quantum theory and its applications [1]. Theory of chemical bonds and main types of solid (metals, semiconductors and dielectrics) are classified according to periodical table of chemical elements [2]. In astrophysics and cosmology, important classifications are the Hertzsprung–Russell diagram for stars and the Hubble tuning fork diagram for galaxies [1]. In Nonlinear Optics, phenomena are classified as terms of a series expansion of the polarization of the medium in terms of the powers of the electric and magnetic field strengths [2]. In Relaxed Optics, the classification of phenomena is carried out according to the main phenomenological characteristics of dynamic processes (corresponding time, energy, and concentration characteristics) in the kinetic concept, and according to the series expansion of the Poynting tensor in the electromagnetic concept [2]. The degrees of complexity of theories can be explored using theory of hybrid systems, according to which there are 10 minimal types systems of knowledge formalization [2].

1. Barrow J. D. Theories of Everything: The Quest for Ultimate. — 2 edition. — Oxford : Clarendon Press, 1991. — 223 p.
2. Trokhimchuck P. P. Theories of Everything: Past, Present, Future. — 1 edition. — Saarbrukken : Lambert Academic Publishing, 2021. — 260 p.

Effect of electric field and mechanical stresses on thermodynamic characteristics of the NH_4HSO_4 ferroelectric within the framework of a two-sublattice pseudospin model

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A modified two-sublattice pseudospin model of NH_4HSO_4 ferroelectrics is proposed, which considers the displacement of sulfate groups in the two-minimum potential well as a pseudospin subsystem [1]. The model takes into account the electrostrictive and piezoelectric coupling of the pseudospin and lattice subsystems. In the mean field approximation, the dielectric, piezoelectric, elastic and thermal characteristics of the crystal are calculated. A satisfactory quantitative description of the relevant experimental data has been obtained. Our model allowed us to describe the effect of hydrostatic pressure on the second order phase transition at the upper Curie point and the first order one at the lower Curie point. We have shown that the distinct first-order phase transition at the lower Curie point as well as the corresponding great changes in lattice strains can be caused by the strong electrostrictive coupling of the pseudospin and lattice subsystems.

Using the Glauber approach, the longitudinal dielectric permittivity of a mechanically clamped crystal and the polarization relaxation times are calculated. It is shown that almost one-time relaxational dielectric dispersion takes place in the crystal. Hydrostatic pressure shifts the dispersion region to higher frequencies. The electric field reduces the relaxation time near the upper Curie temperature.

The calculated change in the crystal temperature under adiabatic application of an electric field, hydrostatic and uniaxial pressures near the lower Curie temperature exceeds 5K.

1. A.S. Vdovych, I.R. Zachek, O.B. Bilenka. Physica B: Condensed Matter, 2024, **695**, p. 416548. https://doi.org/10.1016/j.physb.2024.416548.

Theory of a self-consistent local potential transformation for SPS-type ferroelectrics

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Due to a complex structure and the ability of substitution of the constituent elements, the $Sn_2P_2S_6$-type ferroelectrics (SPS) reveal a plenty of phases and phase transitions at variation of stoichiometry, temperature, pressure, electric field and other external factors (see [1,2] for review). Ionic groups P_2S_6 exist in three configurations, which in the paraelectric phase are described by a symmetrical three-well potential in the energy space [3]. The second order phase transition to the ferroelectric phase occurs due to a dipole ordering of these groups [4]. This insight into the shape of a local potential as well as respective pressure dependences [5] are crucial for our modelling of SPS crystals.

The deformable Blume–Emery–Griffiths (d-BEG) model [6] was proposed to investigate effects of external pressure assuming that the mechanical stress was realized through the lattice strain resulting in restructuring of local atomic configurations. Present investigations of the local potential reshaping is based on the study [7] of mixed-stack compounds with intermolecular electron transfer taking into account electron and phonon subsystems. The last scheme seems to be very promising in our case allowing to reformulate our theory in a self-consistent way providing a unified description for multiply external factors.

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Path integral methods in stochastic equations

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Path integral methods are used to solve stochastic differential equations (SDEs). We consider a stochastic model of many variables given by the SDE system:

$$dX_i(\tau) = A_i(X(\tau))d\tau + \sum_j^n B_{ij}(X(\tau))dW_j(\tau),\ i \in \{1,\dots,n\}.$$

Here we introduce the notation of the stochastic variable $X_i(\tau)$, the Wiener process variables $W_i(\tau)$, $i \in \{1,\dots,n\}$, $\tau \in [t_0, t]$.

The path integral method gives solutions for the conditional probability density of the variables $X_i(\tau)$ in the form of functional quadratures. The solutions are given for the one-dimensional case and for many variables in two forms: "coordinate" variables and "velocity" variables. The two forms of the path integral are related to the methods of their construction. In particular, the "coordinate" form is based on the Wiener measure and the reduction of the SDE to the equivalent equation of constant volatility. The functional integral in the "velocity" variables is obtained on the basis of solving the Fokker–Planck (FP) equation using operator methods and Gaussian functional quadratures. For the one-dimensional case, it is shown that the integrals along the trajectories of both forms are interconnected by the appropriate substitution of variables. Using the example of a functional integral in the "coordinate" form of one variable, it is shown that the conditional probability density satisfies the Chapman–Kolmogorov equation, from which we also obtain the FP equation.

Thermoresponse of structured interface for cell sorting: DPD simulations study

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The cell harvesting on a thermoresponsive interface of PNIPAM polymer has been an active area of research for the last thirty five years. As had been pointed out recently, patterning such surface enables spatial separation and independent tuning of adhesive and repulsive areas of such an interface enhancing cell harvesting and the label-free cell sorting. The formation of structured interface via phase separation of two components, e.g., thermoresponsive PNIPAM and adhesive PGMA have an advantage of lower cost over the lithographic method. However, this process is accompanied with significant polydispersity and large set of parameters which may influence interface functionality. Here the computer simulations may be useful, helping to elucidate which structural properties are more important than the others.

In particular, as was observed in one of the experiments, the thermoresponse of the structured interface can diminish with the increase of the PGMA content. To get more insight into that process, we undertook the DPD simulation of the PNIPAM gel grafted to flat substrate and spherical cap solid PGMA domains, which reflects experimental preparation protocol. We found out that varying the PGMA spherical cap radius, $R_{sp} = 30 - 100$, crosslinking fraction, $\nu = 7, 14\%$, or domains separation, $s = 10 - 40$, influenced the swelling ratio h_1/h_2 of the gel less than increasing the grafting density on the domains to $\rho_{pd} = 0.6$, compared to that on the substrate $\rho_{ps} = 0.2$. Furthermore, we found that lower thermoresponse on the domains due to the higher grafting density can by itself lead to the decrease of swelling ratio for the interface overall. In particular, when the area fraction of domains increased the swelling ratio decreased notably. The study is aimed on finding the optimal conditions for label-free cell sorting. Supported by NAS/ONRG grant 7115, NSF grant 2401713, computing time by NRFU grant 2023.05/0019.

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6-та наукова конференція
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Wednesday, August 27

8:00	Registration
9:00	Opening
9:40	Plenary session
11:00	Conference Photo
11:20	Coffee break
11:40	Plenary session
13:40	Lunch
15:00	Plenary session
17:00	Coffee break
17:20	Plenary session
19:00	Get-together party

Thursday, August 28

9:20	Plenary session
11:20	Coffee break
11:40	Plenary session
13:40	Lunch
15:00	Soft Matter | Complex Systems
16:40	Coffee break
17:00	Soft Matter | Complex Systems
18:00	Poster session
19:30	Conference dinner

Friday, August 29

9:20	Computer Simulations | Quantum Materials and Technologies
11:20	Coffee break
11:40	Computer Simulations | Quantum Materials and Technologies
13:40	Lunch
15:00	Plenary session
17:00	Coffee break
17:20	Plenary session
18:40	Closing

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