**A StatPhys29 satellite conference**

# Statistical Physics in Lviv

**June 30 – July 3, 2025**
**Lviv, Ukraine**

## PROGRAMME AND ABSTRACTS

Lviv – 2025

The Russian war of agression against Ukraine has led to the largest refugee crisis in Europe since WW2, and to very serious disturbances of scientific life in Ukraine. Male scientists below the age of 60 can not cross the state border without special permission, which is not always immediate to obtain. Ukraine has therefore, in addition to all other misfortunes of war, had to face an increased isolation of its scientific community.

The "Statistical Physics in Lviv" satellite conference of StatPhys29 is specifically intended to initiate new connections and broaden and deepen connections already made, and to allow statistical physicists in Ukraine to interact with international colleagues without leaving the country.

The "Statistical Physics in Lviv" conference follows on an online European-Ukrainian conference organized in the framework of the Davydov Readings in December 2023, with the participation of several Board members of the EPS Statistical and Nonlinear Physics Division (EPS-SNPD), and on an upcoming in-person Sweden-Ukraine Conference: Theoretical and Computational Physics, at the Royal Academy of Sciences in Stockholm.

The Conference will consist of invited lectures (40 min) and contributed talks (20 min). Official language of the Conference is English.

## Main topics

- Statistical theory
- Biophysics
- Computer simulations and neural networks
- Quantum information and quantum matter
- Dynamics

## Contacts

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## Sponsoring organizations

- IUPAP through the StatPhys29 regional committee as StatPhys29 satellite conference
- KTH-Royal Institute of Technology (Stockholm, Sweden)
- Institute for Condensed Matter Physics of the NAS of Ukraine (Lviv, Ukraine)
- Bogolyobov Institute for Theoretical Physics of the NAS of Ukraine (Kyiv, Ukraine)
- Interdisciplinary Center for Computer Simulations (Lviv, Ukraine)

## International committee

- Erik Aurell, KTH Royal Institute of Technology, Stockholm, Sweden (co-chair)
- Larissa Brizhik, Bololyubov Institute for Theoretical Physics, Kyiv, Ukraine (co-chair)
- Taras Bryk, Institute of Condensed Matter Physics of NASU, Lviv, Ukraine (co-chair)
- Mats Larsson, Stockholm University, Stockholm, Sweden
- Pawel Horodecki, University of Gdansk, Gdansk, Poland
- Karol Życzkowski, Jagiellonian University, Kraków, Poland
- Angelo Vulpiani, University of Rome “La Sapienza”, Rome, Italy
- Luca Gammaitoni, University of Perugia, Perugia, Italy

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# Programme

**June 30 – July 3, 2025**
**Lviv, Ukraine**

Monday, June 30, 2025

Institute for Condensed Matter Physics of the NASU
Lviv, 1 Svientsitskii Str., Conference hall

14:30 – 14:40 OPENING CEREMONY (E. Aurell, L. Brizhik, T. Bryk)

STATISTICAL THEORY

14:40 – 15:20 J. Kurchan *(Paris, France)*
**The "mosaic" picture of liquids and glasses**

15:20 – 16:00 V. Pergamenshchik *(Warsaw, Poland)*
**Partition function of a 2D hard disk system in terms of the exact free volume: gas, liquid, and in between**

16:00 – 16:30 Coffee Break

16:30 – 17:10 E. Aurell *(Stockholm, Sweden)*
**201 years of Thermodynamics**

17:10 – 17:50 Yu. Holovatch *(Lviv, Ukraine)*
**Emergence of the three-dimensional diluted Ising model universality class in a mixture of two magnets**

17:50 – 18:10 A. Gavrilik *(Kyiv, Ukraine)*
**Tetracriticality and universality classes of Stiefel sigma-models near two dimensions**

18:30 – 21:00 GET-TOGETHER PARTY

Tuesday, July 1, 2025

Institute for Condensed Matter Physics of the NASU
Lviv, 1 Svientsitskii Str., Conference hall

BIOPHYSICS

| | |
|---|---|
| 9:30 – 10:10 | I. Hoffecker *(Stockholm, Sweden)*<br>**Ensemble methods for spatially controlled affinity measurement** |
| 10:10 – 10:50 | A. Baumketner *(Lviv, Ukraine)*<br>**Theoretical studies of protein aggregation** |
| 10:50 – 11:10 | L. Brizhik *(Kyiv, Ukraine)*<br>**Manifestation of coherent many-soliton states in physical and biological systems** |
| 11:10 – 11:40 | Coffee break |
| 11:40 – 12:20 | B. Ostash *(Lviv, Ukraine)*<br>**Ribosome as a regulatory device: a case for antibiotic-producing Streptomyces bacteria** |
| 12:20 – 12:40 | E. Aurell *(Stockholm, Sweden)*<br>**Inferring fitness from large genomic data sets** |
| 12:40 – 13:00 | S. Perepelytsya *(Kyiv, Ukraine)*<br>**Revealing DNA condensation induced by monovalent counterions** |
| 13:00 – 13:20 | M. Samborskyy *(Lviv, Ukraine)*<br>**Oxford nanopore sequencing: at the interface of biology and physics** |
| 13:20 – 14:30 | Lunch |

STATISTICAL THEORY

14:30 – 15:10 K. Życzkowski *(Kraków, Poland)*
**Statistical properties of spectra of typical quantum operations and Lindblad generators**

DYNAMICS

15:10 – 15:50 J. Kurchan *(Paris, France)*
**Time reparametrization softness resolves the dilemma of glass dynamics**

15:50 – 16:20 Coffee break

16:20 – 17:00 P. Cvitanović *(Atlanta, USA; online talk)*
**A field theory of turbulence**

17:00 – 17:20 V. Zasenko *(Kyiv, Ukraine)*
**Advection and diffusion of particles in a random velocity field**

17:20 – 17:40 M. Holovko *(Lviv, Ukraine)*
**On the diffusion of hard sphere fluids in disordered porous media**

17:40 – 18:00 T. Bryk *(Lviv, Ukraine)*
**Transverse dynamics in binary liquids**

19.00 – 21.00 CONFERENCE DINNER

Wednesday, July 2, 2025

Institute for Condensed Matter Physics of the NASU
Lviv, 1 Svientsitskii Str., Conference hall

QUANTUM INFORMATION & QUANTUM MATTER

| | |
|---|---|
| 9:30 – 10:10 | V. Tkachuk *(Lviv, Ukraine)*<br>**Quantum computing of the physical properties of spin systems** |
| 10:10 – 10:50 | P. Horodecki *(Gdansk, Poland)*<br>**TBA** |
| 10:50 – 11:10 | V. Ignatyuk *(Lviv, Ukraine)*<br>**Dependence of the recoherence times and recoherence increments on the state of phonon bath in a single qubit dephasing model** |
| 11:10 – 11:40 | Coffee break |
| 11:40 – 12:00 | E. Aurell *(Stockholm, Sweden)*<br>**Attempts to understand quantum black holes** |
| 12:00 – 12:20 | Kh. Gnatenko *(Lviv, Ukraine)*<br>**Quantum states of spin systems representing bipartite graphs and their study using quantum computing** |
| 12:20 – 12:40 | O. Derzhko *(Lviv, Ukraine)*<br>**Spin-1/2 Heisenberg model on the hyperkagome lattice** |
| 12:40 – 13:20 | A. Sotnikov *(Kharkiv, Ukraine; online talk)*<br>**Tensor network contraction in the zoo of two-dimensional statistical physics models on different Archimedean lattices** |
| 13:20 – 14:30 | Lunch |

COMPUTER SIMULATIONS & NEURAL NETWORKS

14:30 – 15:10 I. Hoffecker *(Stockholm, Sweden)*
**Writing digital data to DNA oligonucleotide barcode networks**

15:10 – 15:30 L. Orellana *(Stockholm, Sweden; online talk)*
**Elastic-network-driven Brownian Dynamics Importance Sampling to track large-scale transitions in sub-mesoscopic protein assemblies**

15:30 – 15:50 T. Patsahan *(Lviv, Ukraine)*
**Adsorption and desorption of cells on micropatterned adhesive surfaces: A Monte Carlo simulation study**

15:50 – 16:20 Coffee break

16:20 – 17:00 A.P. Seitsonen *(Paris, France)*
**Collective dynamics in liquid water from computer simulations using molecular dynamics**

17:00 – 17:20 A. Trokhymchuk *(Ljubljana, Slovenia)*
**Entropy driven bimodality of local density in confined 2D hard disks**

17:20 – 17:40 J. Ilnytskyi *(Lviv, Ukraine)*
**Interaction of colloidal particulates with thermosensitive microstructured polymer brush: dissipative particle dynamics simulations**

Thursday, July 3, 2025

Institute for Condensed Matter Physics of the NASU
Lviv, 1 Svientsitskii Str., Conference hall

STATISTICAL THEORY

10:00 – 10:20 Yu. Kalyuzhnyi *(Ljubljana, Slovenia)*
**Polymerizing hard spheres with double square-well binding potential**

10:20 – 10:40 P. Saprianchuk *(Lviv, Ukraine)*
**A statistical theory of water molecules in narrow carbon nanotubes**

10:40 – 11:00 D. Shapoval *(Lviv, Ukraine)*
**Beyond the epsilon-expansion: reliable critical exponents in structurally-disordered long-range interacting systems**

11:00 – 11:30 Coffee break

11:30 – 12:20 Yu. Slyusarenko *(Kharkiv, Ukraine)*
**Method of canonical transformations in the theory of quantum gases interacting with radiation**

12:20 – 12:30 CLOSING CEREMONY (E. Aurell, L. Brizhik, T. Bryk)

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# Abstracts

**June 30 – July 3, 2025**
**Lviv, Ukraine**

### The "mosaic" picture of liquids and glasses

J. Kurchan

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When a liquid is cooled in such a way that it does not crystallize, it becomes a glass. Ideally, a glass would be a solid phase with no obvious order, an "amorphous solid". The liquid at a temperature just above is described as a fluctuating "mosaic" of fragments of this ideal glass, the larger the closer to the glass transition. Although this sounds plausible, the more one thinks about it, the more elusive this idea becomes. I will describe how, in order to make a meaningful version of these arguments, one is led to a construction essentially equal to image-compression algorithms.

## Partition function of a 2D hard disk system in terms of the exact free volume: gas, liquid, and in between

V.M. Pergamenshchik[a,b], T.M. Bryk[c] and A.D. Trokhymchuk[c,d]

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[b] *Institute of Physics, Academy of Sciences of Ukraine, prospect Nauki 46, 03039, Kyiv, Ukraine*

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[d] *Faculty of Chemistry and Chemical Technology, University of Ljubljana, Večna pot 113, 1000 Ljubljana, Slovenia*

Since nearly two centuries ago van der Waals discovered that molecules have a finite size, there was an idea that the key to the molecular physics is related to the free volume $V_f$ and to solving a hard sphere system. However, this idea has not been converted even to the thermodynamics of a 2D hard disk (HD) system. The first reason is that numerous geometrical constructions, proposed to exactly determine the $V_f$ (surface area available for the disk center in a given state of all other disks), have failed. Second, it is not known how the partition function (PF) depends on $V_f$. In this talk I present the derivation and implementation of the following breakthrough results. The exact formula for $V_f$ is obtained in terms of the intersections of up to five disks of twice the hard-core size; $V_f$ can be computed analytically as a function of $N$ disks' coordinates. The standard "gas" PF $Z_G\{V_f\}$ is obtained as a functional of $V_f$; For high "liquid" packing fractions $\eta > 0.55$ when $V_f$ is small, the $Z_G$ crossovers into the "liquid" PF $Z_L = V_f^N$. These formulae were used to analytically convert the configurations, generated in our MC simulation, to the $Z$, entropy, and pressure $P$ for $\eta$ up to the close packing $\eta_{cp} = 0.907$. Comparing our $P$ to the known numerical pressure $P_{\rm exp}$, we found three distinctive regimes which we conventionally call gas, liquid, and mix-liquid regimes (the two-phase coexistence region $0.69 < \eta < 0.72$ is not considered). In the gas regime, $\eta < 0.51$, $P_{\rm exp}$ is reproduced by the "gas" PF $Z_G$. In the liquid regime, $0.72 < \eta < \eta_{cp}$, $P_{\rm exp}$ is reproduced by the $Z_L$. In the intermediate mix-liquid regime, $0.55 < \eta < 0.69$, the system is a mixture of the HDs at actual $\eta$ and defects in the form of HDs caged at $\eta = 0.68$, which are precursors of the nascent hexagonal order. Here the $P_{\rm exp}$ is reproduced by the $P_L$ for the mixture.

### 201 years of Thermodynamics

E. Aurell

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In 1824 Nicolas Léonard Sadi Carnot was a 28-year old engineer, part-time employed as lieutenant by the French General Staff. His military duties were not very time-consuming, partly surely because his father Lazare Carnot had been a leading revolutionary, and Napoleon's last minister of interior, and the newly restored French monarchy was, for obvious reasons, wary of Carnot junior. In his spare time, which was probably most of his time, he became interested in steam engines. These were then already widely used, and it was well known that the British could build more efficient engines than the French.

Trying to understand why this was so, Carnot wrote a memoir *Réflexions sur la puissance motrice du feu et sur les machines propres à développer cette puissance*, often today referred to as Carnot's *Treatise on Heat*, which he published in 600 copies, printed at his own expense. This event counts as the beginning of thermodynamics, the science about which Einstein famously said that it is the only one of universal content which will never be overthrown. Thirty-two years later Rudolf Clausius gave his statement of the Second Law.

Building on the bicentennial conference held in September last year in Paris I will give a glimpse of what Carnot and Clausius actually did and wrote, and how they presented it, and try to explain why the science of thermodynamics continues to play such a large role in Physics. I will also highlight the theory of irreversibility and non-equilibrium entropy of the late mathematical physicist Göran Lindblad, and how they connect to problems of very recent concern in stochastic thermodynamics and quantum thermodynamics.

### Emergence of the three-dimensional diluted Ising model universality class in a mixture of two magnets

J.J. Ruiz-Lorenzo[a], M. Dudka[b,c,d], M. Krasnytska[b,c], and Yu. Holovatch[b,c,e,f]
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[b] *Institute for Condensed Matter Physics of the National Academy of Sciences of Ukraine, 1 Svientsitskii Str., 79011 Lviv, Ukraine*
[c] $\mathbb{L}^4$ *Collaboration & Doctoral College for the Statistical Physics of Complex Systems, Leipzig-Lorraine-Lviv-Coventry, Europe*
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[e] *Centre for Fluid and Complex Systems, Coventry University, Coventry, CV1 5FB, United Kingdom*
[f] *Complexity Science Hub, 1030 Vienna, Austria*

Usually, the impact of structural disorder on the magnetic phase transition in the 3D Ising model is analyzed within the framework of quenched dilution by a non-magnetic component, where some lattice sites are occupied by Ising spins, while others are non-magnetic. This kind of quenched dilution, according to the Harris criterion, leads to a change in the critical exponents that govern the asymptotics in the vicinity of the phase transition point. However, the inherent reason for the emergence of a new, random Ising model universality class is not the presence of a non-magnetic component but the disorder in structure of spin arrangement. To demonstrate this fact we consider a random mixture of two Ising-like magnets that differ in spin length $s$ and concentration $c$. In doing so, we analyze the effect of structural disorder *per se* without appealing to the presence of a non-magnetic component. We combine functional integration and field-theoretical renormalization group methods with extensive numerical simulations to demonstrate the emergence of the 3D randomly diluted Ising model universality class in a random mixture of two Ising magnets. While the asymptotic critical exponents coincide with those known for the site-diluted 3D Ising model, the effective critical behavior is triggered by parameters $s$ and $c$. The impact of their interplay is a subject of detailed analysis.

1. J. J. Ruiz-Lorenzo, M. Dudka, M. Krasnytska, Yu. Holovatch. Phys. Rev. E **111** (2025) 02412.
2. M. Dudka, M. Krasnytska, J. J. Ruiz-Lorenzo, Yu. Holovatch. JMMM **575** (2023) 170718.

## Tetracriticality and universality classes of Stiefel sigma-models near two dimensions

A. Gavrilik and A. Nazarenko

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There exist miriads of real physical systems exhibiting tetracritical behavior. However, their systematization in terms of universality classes, unlike bi-critical systems, i s still lacking. A possible step to fill this gap is suggested by a class of unconventional nonlinear sigma-models (NLSMs) – namely Stiefel sigma-models. Note, a simpler examples of NLSMs are well-known (see e.g. [1,2]: those involve single charge (one coupling constant), and can describe bi-critical systems only. Situation with Stiefel sigma-models is principally different, as it was noticed in [3].

Within the NLSMs on real Stiefel manifolds $SO(N)/SO(N-k)$, using one-loop renormalization and the analysis of scaling behavior, a new infinite series of universality classes of tetra-critical systems with orthogonal symmetry have been derived [4]. The Stiefel NLSMs incorporate orthogonal and Grassmann subsystems of Goldstonions, what implies two competing order parameters. The universality classes in that series are identified by the respective (tetra)critical points and depend on $N$, $k$ and $\epsilon = d-2$. These findings are of basic novelty and suggest theoretical groundwork that could be very helpful for better understanding and systematizing diverse complex phenomena, including possibly the realm of high-temperature superconductivity.

1. E. Brezin, J. Zinn-Justin, Renormalization of the nonlinear $\sigma$ model in $2+\epsilon$ dimensions — Application to the Heisenberg ferromagnets. Phys. Rev. Let. 36, 691 (1976).
2. S. Hikami, Renormalization group functions of orthogonal and symplectic non-linear $\sigma$ model. Prog. Theor. Phys. 64, 1466 (1980).
3. A.M. Gavrilik, Self-interaction anisotropy of Stiefel systems of Goldstonions. Mod. Phys. Lett. A 4, 1783 (1989).
4. A.M. Gavrilik, A.V. Nazarenko, Scaling behavior and phases of nonlinear sigma model on real Stiefel manifolds near two dimensions. Universe 11(4), 114 (2025); https://doi.org/10.3390/universe11040114

**Ensemble methods for spatially controlled affinity measurement**

I. Hoffecker and B. Högberg

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Multivalent interactions are central to the function of many biomolecular systems, particularly in antibody-antigen binding, where spatial arrangement of epitopes dictates the balance between monovalent and bivalent engagement. However, conventional methods for affinity measurement such as ELISA or SPR do not resolve spatial effects, conflating true affinity with avidity and offering limited insight into the underlying interaction states.

Here, we present ensemble-based methods for measuring and modeling antibody binding to spatially patterned antigens using DNA origami nanostructures. By precisely varying inter-antigen distances and quantifying equilibrium binding using colorimetric assays, we derive "avidity profiles"—compact, interpretable parameter sets that capture how multivalent binding modes depend on spatial constraints.

We employ steady-state occupancy measurements and Markov modeling to deconvolve ensemble binding into its constituent states, revealing how proximity-driven bivalent binding competes with steric hindrance and saturating monovalent interactions. This framework introduces two spatially dependent dissociation constants to characterize transitions between binding modes and incorporates them into a predictive model grounded in physical rate laws.

Together, these results demonstrate how spatial patterning, ensemble measurements, and statistical physics models can jointly reveal the geometry-dependent behavior of antibodies. The approach provides a foundation for understanding multivalent binding in complex environments and could be extended to more disordered antigen landscapes using stochastic geometry and integrative modeling techniques.

### Theoretical studies of protein aggregation

A. Baumketner

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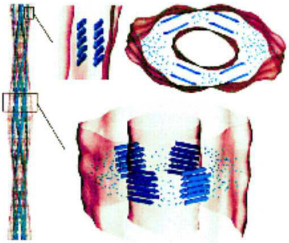

Protein aggregation refers to the proces of selfassembly of fully or partially unfolded proteins that leads to the formation of large insoluble complexes, aggregates. One type of protein aggreates — amyloid fibrils is implicated in various neurodegenertive diseases and also has found multiple uses in technology. We will discuss what can be learned about amyloid using theoretical models and methods. We will start with a broad overview of problems and challenges facing theoretical approaches, from the description of small oligomers [1], which are often considered kinetic intermediates to fibrils, to particlar details of amyloid structure [2]. Then we will focus on aggregation pathway of the peptide involved in Alzheimer's disease, A$\beta$ [3]. Finally, we will present a model specifically designed for simulation of protein aggregates [4] and discuss the effect of electric field on amyloid assembly [5].

1. A. Baumketner and J. E. Shea, Biophysical Journal **89**, 1493 (2005).
2. L. Negureanu and A. Baumketner, Journal of Molecular Biology **389**, 921 (2009).
3. A. Baumketner, M. G. Krone, and J. E. Shea, Proceedings of the National Academy of Sciences of the United States of America **105**, 6027 (2008).
4. B. Ni and A. Baumketner, Journal of Chemical Physics **138**, 064102 (2012).
5. A. Baumketner, Journal of Physical Chemistry B **118**, 14578 (2014).

**Manifestation of coherent many-soliton states in physical and biological systems**

L. Brizhik

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There is a large class of quasi-one-dimensional molecular structures in physical and biological systems with moderately strong electron-phonon interaction. The latter leads to self-trapping of quasiparticles in the state known as Davydov's soliton. In the general case soliton parameters are determined by the constant, which plays the role of the dimensionless nonlinearity constant in the cubic nonlinear Schroedinger equation and is defined by the exchange (resonant) electron energy, lattice elasticity and electron-phonon interaction constant. Although this equation always admits soliton solution, according to the inverse scattering method the initial excitation can evolve with time into the linear excitations, soliton or many-soliton states. This is determined by the corresponding physical conditions.

In biological systems energy of the ATP hydrolysis can be enough to excite not more than one or two solitons which have no spin and can be bound in the bisoliton state. In polymers and in macromolecules in the electron transport chain in the Krebbs cycle solitons are formed by electrons. The lowest energy bound state of two electrons is a bisoliton which can be formed by two electrons with opposite spins. It is shown that two electrons with parallel spins form a triplet soliton state, which has higher energy than a bisoliton. According to the Hall effect measurements, in the Krebbs cycle in Cyt-C oxidase which possesses strong local magnetic field, electrons are transported one by one, corresponding to the triplet state, while in other enzymes without magnetic field electrons are transported by pairs, corresponding to bisolitons.

In conducting quasi-one-dimensional systems a large number of free electrons (holes) can exist. In such a case they can self-trap in a many-soliton state in the form of the cnoidal wave if their number is lower than the critical value, or remain in the delocalized state in the form of a plane wave at a bigger concentration (cf. HTSC, SC of organic systems).

**Acknowledgment**

The work is supported by the project PK 0122U000887 of the NASU and by Simons Foundation grant SFI-PD-Ukraine-00014573.

## Ribosome as a regulatory device: a case for antibiotic-producing Streptomyces bacteria

B. Ostash and V.-M. Tseduliak

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The ribosomal synthesis of proteins (translation) is an evolutionary refined balance between the speed and accuracy. That balance can be dramatically shifted, either pharmacologically or genetically, to the degree incompatible with cell survival. This insight came first in 1960s with the isolation of *Escherichia coli* mutants deficient in gene *rpsL* for ribosomal protein S12. Since then missense mutations within *rpsL* provided an invaluable window into molecular details of protein synthesis. In the focus of our research is bacterial genus Streptomyces renowned for its ability to produce numerous specialized metabolites of immense practical value, such as antibiotics. The introduction of *rspL* mutations into streptomycete genomes is often a part of strain improvement programs, although it remains unclear as to why such mutations boost metabolism. Using *Streptomyces albidoflavus* J1074 as a model species, we generated isogenic rpsL mutant lines carrying substitutions Lys88Asp, Lys88Arg and Arg94Gly, and characterized their properties. Our major finding is that *rpsL* mutations per se might be not a cause of the improved phenotype, but their combination with the other, often unknown, mutations underlie these favorable changes. The occurrence of these unanticipated mutations can be viewed as a compensation for the fitness losses incurred by the initial *rpsL* mutations. Our results suggest that the initial disadvantages caused by rpsL mutations can have something to do with the synthesis of second nucleotide messenger c-di-GMP, one of the most versatile mediators of physiological processes in *Streptomyces*. To gain deeper insight into regulatory function of *rpsL* mutations, we initiated cryo-EM reconstruction of ribosome structures from the wild type strain and aforementioned mutants.

**Inferring fitness from large genomic data sets**

E. Aurell

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Throughout the course of the SARS-CoV-2 pandemic, genetic variation has contributed to the spread and persistence of the virus. For example, various mutations have allowed SARS-CoV-2 to escape antibody neutralization or to bind more strongly to the receptors that it uses to enter human cells. In the course of the pandemic more viral genomes (tens of millions) were produced than in any previous pandemic, which can then be used in ways that could not be envisaged in the past.

I will discuss what such data can look like, and how one can visualize mutation frequencies at each position along the genome with a time resolution down to a week for some restricted geographic regions such as the UK. I will further discuss two methods to infer genetic fitness (additive and epistatic fitness) from such data sets, and compare them to simulations where underlying parameters are known. I will also review earlier work on the topic with Simona Cocco and Rémi Monasson, and very relevant related work by Martin Weigt and coworkers.

This is partially joint work with Hongli Zeng and John Barton and others, published in Physical Biology 22:016003 (2024).

### Revealing DNA condensation induced by monovalent counterions

T. Bubon, D. Piatnytskyi, and S. Perepelytsya

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In aqueous solutions, the DNA macromolecule carries a net negative charge, with each phosphate group in the double-helix backbone bearing a single negative charge (-1e). This negatively charged backbone is neutralized by positively charged ions (counterions) from the solution. At sufficiently high concentrations, counterions can induce the formation of stable DNA-DNA contacts, leading to macromolecular condensation [V.A. Bloomfield, Biopolymers 44, 269 (1997)]. Experimental data show that DNA condensation typically occurs in the presence of trivalent (3+) and higher-charged ions. In the case of divalent counterions, condensation is observed only under specific conditions and for certain nucleotide sequences. For monovalent ions, condensation was generally considered unlikely, as polyelectrolyte models predict that the electrostatic attraction between DNA molecules surrounded by monovalent ions is too weak to drive condensation [J. Ray, G.S. Manning, Langmuir 10, 2450 (1994)].

In this work, we present a molecular dynamics and quantum chemical study of DNA in the presence of monovalent $Li^+$, $Na^+$, and $K^+$ ions. These ions have different character of hydrated, and their interaction with the phosphate groups plays a crucial role. Condensation of DNA was observed in the case of $Li^+$, while no condensation occurred with $Na^+$, and $K^+$ ions. A key feature is that the hydration shell of $Li^+$ typically consists of four water molecules arranged in a tetrahedral structure. Upon interaction with the phosphate group of the DNA double helix, one water molecule is substituted by an oxygen atom from the $PO_4^-$ group. In the case of a DNA–$Li^+$–DNA contact, two water molecules are replaced by oxygen atoms from the phosphate groups of two adjacent DNA strands. The contribution of hydration to the interaction energy stabilizes DNA–DNA contacts, thereby facilitating condensation.

The obtained results are important for understanding the structure of DNA gels in the presence of LiCl and the dynamics of ions under an external electric field. These findings can be applied to the design and improvement of lithium-ion supercapacitors that use DNA-based electrolytes [S.B. Mitta *et al.*, Advanced Materials Interfaces 9, (2022)].

**Oxford nanopore sequencing: at the interface of biology and physics**

M. Samborskyy

*Explogen LLC, 20 Zelena Street, Lviv, 79005, Ukraine,*
*E–mail: marko@explogen.com.ua*

With the rapid progress of sequencing technologies over the last decades, and all the impact it is having at the sphere of biotechnology and medicine, come some quite interesting technical challenges that we need to solve in order to be able to get most from the available technology and data that it's generates. After a brief introduction of sequencing and main differences between three main generations of sequencing technologies to non-biologists, we would delve into some technical peculiarities of Oxford Nanopore Sequencing Technology and practical implications for the application of this technology, such as:

1. Molecular physics of nanopore sequencing and requirements for sample purity to reduce pore blocking by co purified polymers or DNA modifications that can get stuck in pore;

2. Signal sensing from nanopores and challenges in Signal to Noise ratio when sensing currents in the $10^{-11}$–$10^{-10}$ Amp range with voltage across the pore in the region of 170 mV – 250 mV;

3. ONT signal trace basecalling challenges (due to 5–20 adjacent bases having an impact on the signal level) and application of latest AI models for ONT data processing (LSTM and Transformers).

### Statistical properties of spectra of typical quantum operations and Lindblad generators

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Dynamics of open quantum systems is analyzed under the assumption of discrete or continuous time evolution. We introduce ensembles of random quantum operations and random Lindblad generators, each parameterized by a point in a unit cube. Three axes $(q, b, r)$ of both cubes correspond to the quantumness parameter $q$, characterizing the process of decoherence and governing the transition from quantum to classical, the parameter $b$ describing breaking of the detailed balance condition, which implies that the spectrum of the operator is real, and the rescaled rank $r$ of the operator. The corner $(1, 1, 1)$ of the 3-cube represents standard ensembles of generic random quantum operations and random Lindblad generators. Proposed random matrix models allow us to analyze the influence of these three physical parameters for the statistical properties of complex spectra of the corresponding operators.

*Joint work with* Wojciech Tarnowski (Cracow), Dariusz Chruściński and Sergey Denisov (Oslo).

**Time reparametrization softness resolves the dilemma of glass dynamics**

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Time reparametrization softness is the property that a system's dynamics may change dramatically their pace under a weak appropriate perturbation. It has long been recognized as central to the glass phenomenology (although seldom with that name), and more recently as a mechanism whereby a 'gravity'-like low energy limit arises in some quantum systems, such as the SYK (Sachdev–Ye–Kitaev) model. It has now been recognized as resolving the dilemma of whether glasses are purely dynamic, or the consequence of static thermodynamic features. The answer is 'both'.

### A field theory of turbulence

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Gutzwiller semi-classical quantization, Boven-Sinai-Ruelle dynamical zeta functions for chaotic dynamical systems, statistical mechanics partition functions, and path integrals of quantum field theory are often presented in ways that make them appear as disjoint, unrelated theories. However, recent advances in describing fluid turbulence by its dynamical, deterministic Navier-Stokes underpinning, without any statistical assumptions, have led to a common field-theoretic description of both (low-dimension) chaotic dynamical systems, and (infinite-dimension) spatiotemporally turbulent flows.

I will use a lattice discretized field theory in 1 and 1+1 dimensions to explain how temporal 'chaos', 'spatiotemporal chaos' and 'quantum chaos' are profitably cast into the same field-theoretic framework.

For in-depth dive, see `ChaosBook.org/overheads/spatiotemporal`

**Advection and diffusion of particles in a random velocity field**

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A tractable model is used to investigate particle transport mechanisms – advection and diffusion – in a random two-dimensional velocity field. Diffusion is associated with short correlation times of the velocity field, while advection dominates for longer correlation times. A unified theoretical framework is developed to describe transport across the entire range of correlation times. The core of the approach is the transformation from the Eulerian to the Lagrangian velocity correlation function, enabling a new closure scheme for the statistical transport equations. The model's predictions are validated through direct numerical simulations. Simulation results show agreement with the theoretical solutions, confirming the approach's consistency and applicability.

### On the diffusion of hard sphere fluids in disordered porous media

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We proposed a new extended version of Enskog theory for the description of the self-diffusion coefficient of a colloidal hard-sphere fluid adsorbed in a matrix of disordered hard-sphere obstacles [1]. In the formation of the input information for this theory we try to take into account that matrix particles are immobile and fluid particles are mobile. 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 in random porous media strongly correlate with ration of thermodynamic porosity to geometrical porosity previously introduced by us in the description of thermodynamical properties of hard-sphere fluid in porous media [2]. This ration is interpreted as the fraction of volume free matrix particles and from fluid particles trapped by matix particles. It is shown that the introduction of this volume fraction by the Fermi-like distribution leads to the best agreement between theoretical prediction and computer simulation results [3].

1. Holovko M.F., Korvatska M.Ya., Condens. Matter Phys., 2025, (in press).
2. Holovko M., Patsahan T., Dong W., Cond. Matter Phys, 2017, **20**, 33602.
3. Chang R., Jagannathan K., Yethiraj A., Phys. Rev. E, 2004, **69**, 051101.

### Transverse dynamics in binary liquids

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Transverse collective excitations in 50–50 and 80–20 Lennard-Jones binary liquid mixtures are studied for different mass ratio of components $R$ at fixed numerical densities. Increasing the mass ratio results in a growing difference between frequencies of shear waves and transverse optic modes. We report an increase in the propagation gap width for shear waves with mass ratio of components and compare it to the gap width expression, known from the transverse dynamics of simple liquids. A four-variable dynamic model [1] of transverse dynamics in binary liquids with an account of cross correlations between total-mass and mass-concentration transverse current fluctuations is solved analytically in the long-wavelength region. An equation for the propagation gap of shear waves for binary liquids is reported and analyzed.

1. T. Bryk, M. Kopcha, I. Yidak. *J. Chem. Phys.* **161** 184505 (2024).

### Quantum computing of the physical properties of spin systems

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In this talk, we present methods for studying the dynamical and thermodynamic properties of spin systems using quantum computers. The time evolution of the expectation value of an operator that commutes with the Hamiltonian is determined by the energy level spacings. When an operator exists that anticommutes with the Hamiltonian, the energy spectrum becomes symmetric under energy inversion. This symmetry is related to the supersymmetry (SUSY) of the Hamiltonian. In such cases, the time evolution of the expectation value of the anticommuting operator is governed by the energy levels. Based on this property, we propose a quantum algorithm for detecting energy levels. We further generalize this approach to cases where the Hamiltonian does not exhibit SUSY, using ancilla qubits. The method is implemented on IBM quantum computers and demonstrates good performance and resilience to noise.

A major challenge in studying the thermodynamic properties of quantum systems and computing the partition function lies in simulating the Boltzmann factor on a quantum computer, as it is a non-unitary operator. As quantum computers operate via unitary transformations, it is, in principle, possible to simulate the evolution of quantum systems using quantum gates. We implement the Boltzmann factor of the Ising model on a quantum computer by expressing it as the trace of an evolution operator, defined by an effective Hamiltonian, over ancilla qubits. This connection between the evolution operator and the Boltzmann factor allows us to compute the partition function of the Ising model on a quantum computer, including versions of the model with complex parameters. This, in turn, enables the study of Fisher and Lee-Yang zeros. Moreover, this realization of the Boltzmann factor also allows us to determine the ground state of a spin system, specifically in the case of the Ising model As an example, the partition function of a two-spin Ising cluster is calculated using the IBM quantum computer. The ability to determine the ground state is also demonstrated for this two-spin cluster. The results obtained from the quantum computer are in good agreement with theoretical predictions.

**Dependence of the recoherence times and recoherence increments on the state of phonon bath 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, there appears the correlational contribution to the generalized decoherence function of a very interesting nature [3–4]: it 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 $\gamma_{\text{extr}}$ are studied as the functions of coupling strengths $\lambda$, ohmicity indexes $s$ and temperature $T$. We found that the sub-Ohmic and Ohmic regimes are more preferable for the recoherence than the super-Ohmic one. The most interesting observation is that the short time behaviour (the system recoherence) 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 $\gamma_{\text{extr}}$ in some sense.

1. V.G. Morozov, S. Mathey and G. Röpke, Phys. Rev. A **85**, 022101 (2012).
2. H.-P. Breuer and F. Petruccione, *The Theory of Open Quantum Systems* (Oxford University, Oxford, 2002).
3. V. V. Ignatyuk, V. G. Morozov, Phys. Rev. A **91**, 052102 (2015).
4. V. V. Ignatyuk, Phys. Rev. A **92**, 062115 (2015).

### Attempts to understand quantum black holes

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The quantum Nature of black holes is a fundamental problem in Physics. One way to see that this is so is to realize that the most conservative solutions to the problem rely on there being a theory of quantum gravity. Such a theory does not exist, or at least not one that is experimentally tested and widely accepted. Another reason is that Hawking's theory of Hawking radiation leads to the Bekenstein-Hawking entropy of black holes which is super-extensive *i.e.* increases faster than linearly with mass. This is highly exotic behaviour for entropy.

I will discuss a pedestrian attempt to this problem where I consider pairwise entanglement and subsystem entropy in a family of ensembles of random pure Gaussian states. The additional assumption of Gaussianity makes it possible to go beyond Page's classical result on average subsystem entropy, and compute averages in ensembles constrained by given marginals. I will estimate average subsystem entropy which shows a kind of thermalization, and how much pairwise entanglement there is on average among the modes in this model.

This is in joint work with Lucas Hackl, Paweł Horodecki, Robert Jonsson and Mario Kieburg, available as Physical Review Letters 133:060202 (2024) and [arXiv:2505.03696].

**Quantum states of spin systems representing bipartite graphs and their study using quantum computing**

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Progress in quantum technologies has intensified interest in the development of new quantum algorithms for studying fundamental problems and solving practical tasks using quantum programming. We consider spin systems with different types of interactions and examine their evolutionary states through analytical methods as well as quantum programming [1]. Quantum protocols for preparing evolutionary quantum states, which can be represented by bipartite graphs, are constructed. We analyze the properties of these states—such as entanglement distance and quantum correlators in the states—both analytically and using quantum computing. The results of quantum calculations are in agreement with the theoretical ones.

Additionally, we discuss the problem of determining the parameters of Hamiltonians for spin systems through quantum programming. The obtained results open up the possibility of examining the properties of graphs using quantum technologies.

1. Kh. P. Gnatenko, Eur. Phys. J. Plus. Vol. 140, No. 3. Art. 241. 7 p (2025).

### Spin-1/2 Heisenberg model on the hyperkagome lattice

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The $S=1/2$ Heisenberg model on the hyperkagome lattice (three-dimensional network of corner-sharing triangles) is among the standard systems in the theory of frustrated quantum magnets. For the antiferromagnetic sign of exchange interaction it allows us to demonstrate the interplay of geometrical frustration and quantum fluctuations in the ground state, whereas for the ferromagnetic one it enables to reveal the effect of frustration at finite temperatures.

In this contribution, I intend to present our findings for both signs of the exchange interaction: $J>0$ and $J<0$, $|J|=1$, for more details see Refs. [1,2]. Thus, according to the entropy-method interpolations and the finite-temperature Lanczos method calculations for the hyperkagome-lattice $S=1/2$ Heisenberg *antiferromagnet*, the ground-state energy $e_0$ is expected to lie between $-0.441$ and $-0.435$, low-lying excitations are gapless and the specific heat $c(T)$ decays as $T^2$ when $T \to 0$, the uniform susceptibility $\chi(T)$ is around 0.1 at $T=0$, and $c(T)$ exhibits a low-temperature peak at $T<0.05$, i.e., well below the main high-temperature peak at $\approx 0.67$ [1]. More methods are available for the hyperkagome-lattice $S=1/2$ Heisenberg ferromagnet: Spin wave theory, double-time temperature Green's function method, high-temperature series analysis, or quantum Monte Carlo simulations. According to our calculations for the hyperkagome-lattice *ferromagnet*, the Curie temperature $T_c$ is about 0.33 and $c(T)$ exhibits a shoulder above $T_c$ [2]. A combined view and comparison to the diamond-lattice case – another three-dimensional lattice with the same coordination number 4, but bipartite one – allows us to illustrate the effect of lattice geometry on thermodynamic properties of the quantum Heisenberg model.

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

1. T. Hutak *et al.*, *Phys. Rev. B* **110**, 054428 (2024).
2. M. Parymuda, T. Krokhmalskii, and O. Derzhko, Institute for Condensed Matter Physics of the National Academy of Sciences of Ukraine, preprint ICMP-24-03E (2024).

**Tensor network contraction in the zoo of two-dimensional statistical physics models on different Archimedean lattices**

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We develop a new methodology to contract tensor networks within the corner transfer matrix renormalization group approach for a wide range of two-dimensional lattice geometries. We discuss contraction algorithms on the example of triangular, kagome, honeycomb, square-octagon, star, ruby, square-hexagon-dodecahedron, and dice lattices.

As benchmark tests, we apply the developed method to the classical Ising model on different lattices and observe a remarkable agreement of the results with the available from the literature [1]. The approach also shows the necessary potential to be applied to various quantum lattice models in a combination with the wave-function variational optimization schemes.

The work is supported by the National Research Foundation of Ukraine in the framework of the call "Excellent science in Ukraine" 2024–2026, project No. 0124U004372.

1. I.V. Lukin and A.G. Sotnikov, Corner transfer matrix renormalization group approach in the zoo of Archimedean lattices, Phys. Rev. E 109, 045305 (2024).

### Writing digital data to DNA oligonucleotide barcode networks

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DNA has been proposed as a medium for data storage in answer to the growing urgency for increasing the world's data storage capacity. While sequencing costs have exponentially fallen with years, the combined logistical and economic hurdles of novo DNA synthesis make the writing step of storage via DNA still impractical. DNA based networks have been used in spatial biology to preserve and retrieve the distributions of molecules in tissues via sequencing based information. The networks operate by a principle of spatial coherence, in which proximity-dependent associations between locally amplified, randomly tagged DNA molecules, creates a well defined relationship between network and Euclidean space, enabling inference of the latter via structural analysis of the former. Here we invert this principle for the purposes of DNA data storage and show how selective partitioning of spatial DNA networks may be used to preserve ordinal relationships required in storing bit strings, allowing for data writing to be conducted with random, bulk synthesized DNA instead of custom de novo synthesis. This approach could reframe the problem of DNA based data storage and open up new avenues of low cost and on-demand writing.

**Elastic-network-driven Brownian Dynamics Importance Sampling to track large-scale transitions in sub-mesoscopic protein assemblies**

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Protein conformational changes are the cornerstone of biological function, executing and regulating almost all life processes. Although conformers captured by structural techniques represent metastable states, the pathways connecting them have been elusive for both experiments and simulations [1]. Nowadays, cryogenic Electron Microscopy is providing rich structural data on proteins trapped in different states for increasingly large systems, but these are out of scope for current modelling methods, which usually exhibit an N2 dependence on size. Here we present an overview of coarse-grained and atomistic methods to sample protein conformational spaces, introducing eBDIMS2, an optimized version with quasi-linear size dependence. Based on our previous eBDIMS algorithm (ENM-driven Brownian Dynamics Importance Sampling) [2], eBDIMS2 [3] is able to simulate on a desktop computer exceptionally complex transitions for megadalton protein assemblies, like the rotary motion of ATP synthases. Not only eBDIMS2 pathways spontaneously visit experimentally trapped intermediates but also overlap with microsecond Molecular Dynamics simulations requiring extensive supercomputing resources. By integrating Elastic Networks with Brownian Dynamics, eBDIMS2 allows an unprecedented exploration of conformational changes of sub-mesoscopic systems, previously inaccessible.

1. Orellana L., "Large-scale conformational changes and protein function", Frontiers in Molecular Biosciences, 2019
`https://doi.org/10.3389/fmolb.2019.00117`
2. Orellana et al., "Prediction and validation of protein intermediate states and transition pathways from structurally-rich ensembles and coarse-grained simulations", Nat. Communications, 2016
`https://doi.org/10.1038/ncomms12575`
3. Scaramozzino et al., "Breaking the size limit: efficient sampling of large-scale transition pathways and intermediate conformations in sub-mesoscopic protein complexes", Nat. Communications
`https://doi.org/10.21203/rs.3.rs-6504036/v1`
(awaiting resubmission).

### Adsorption and desorption of cells on micropatterned adhesive surfaces: A Monte Carlo simulation study

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Affinity-based cell sorting at micropatterned surfaces relies on the differential adhesion of cells to spatially structured substrates. In such systems, adsorption and desorption processes are governed by the physicochemical properties of the surface patterns, such as domain size, shape, spacing, and adhesion energy. Although the efficiency of cell adsorption and desorption depends on the interplay of these characteristics, understanding the individual contribution of each parameter remains essential. In this study, we investigate how the size of adhesive domains affects the detachment of adsorbed cells, depending on the strength of the repulsive force exerted by a thermoresponsive polymer filling the inter-domain space. To this end, we propose a model capable of describing cell adhesion to and detachment from a microstructured surface containing randomly distributed adhesive domains. Monte Carlo simulations are performed for this model over a range of domain sizes, while keeping the surface coverage fraction of adhesive domains fixed. Although the model is intentionally idealised, it enables a clear assessment of how the aforementioned geometric features affect sorting efficiency.

## 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.

1. N March & M Parrinello, *Collective Effects in Solids and Liquids*, Adam Hilger Ltd, Bristol (1982).
2. G Ruocco & F Sette, *Condens Matter Phys* **11**, 29 (2008).
3. T Bryk & A P Seitsonen, *Cond Matt Phys* **19**, 23604 (2016).
4. G R Medders & F Paesani, *Infrared and Raman Spectroscopy of Liquid Water through "First-Principles" Many-Body Molecular Dynamics*, J Chem Theory Comput **11**, 1145 (2015).
5. D P Kovács *et al.*, *arXiv* 2312.15211 (2023).
6. M de la Puente & D Laage, *J Amer Chem Soc* **145**, 25186–25194 (2023).

**Entropy driven bimodality of local density in confined 2D hard disks**

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By combining computer simulations and a unit cell model approach, we report an observation [1] of the apparent bimodal probability distributions of local structural ordering and local density in a two-dimensional (2D) hard disk array confined laterally within a quasi-1D hard wall channel. The observed feature aligns with the concept of locally favored structures developed in studies of the anomalous thermodynamic and kinetic behavior of hydrogen-bonding fluids, except that the case reported here is driven by entropic bonding only. The bimodality is observed in a range of densities associated with those before the freezing in bulk 2D hard disks. It indicates a crossover from the "gas-like" to "liquid-like" state in confined quasi-1D hard disks. This phenomenon was not reported yet for bulk 2D hard disks and is physically unexpected for confined q1D hard disks. The presence of the "gas-liquid" crossover in bulk 2D hard disks is discussed.

1. Trokhymchuk, A., Huerta, A., Bryk, T., Bimodality of local structural ordering in extremely confined hard disks, *J. Chem. Phys.* **162**, 184504 (2025).

**Interaction of colloidal particulates with thermosensitive microstructured polymer brush: dissipative particle dynamics simulations**

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Microstructured surfaces composed of adherent domains and stimuli-responsive polymer domains (that undergo swelling-shrinking upon stimuli, e.g., temperature change around the low critical solution temperature, LCST) were proven to catch and release colloidal particulates (CP) effectively. Such structures have the advantage over just uniform stimuli-responsive surfaces because, on the microstructured surface, sticky and pushing-off properties are decoupled so that the properties of each domain can be adjusted 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. The study is relevant and motivated by the problems of harvesting and sorting prokaryotic and eukaryotic cells on microstructured surfaces.

1. J. Ilnytskyi, D. Yaremchuk, S. Minko, Interaction of Colloidal Particulates with Dynamic Microstructured Polymer Brushes: Computer Simulations, Langmuir 2025, 41, 20, 12731–12744, DOI: 10.1021/acs.langmuir.5c00929

**Polymerizing hard spheres with double square-well binding potential**

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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 $\sigma$. 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.

1. J. Rescic, Y.V. Kalyuzhnyi, P.T. Cummings, *J. Phys.: Cond. Mat.* **28**, 414011 (2016).

2. Y.V. Kalyuzhnyi, H. Docherty, P.T. Cummings, *J. Chem. Phys.* **135**, 014501 (2011).

### A statistical theory of water molecules in narrow carbon nanotubes

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Recently, it was argued that the water molecules encapsulated into a single-wall (6,5) carbon nanotube exhibit a temperature-driven pseudo-phase transition around 150 K [1]. This transition was interpreted as a change in the water dipole orientation with respect to the nanotube axis. Motivated by these experiments, we performed quantum chemistry calculations, molecular dynamics simulations and elaborated a simple lattice model which accounts for short- and long-range interactions as well as rotation in a narrow tube that provides statistical mechanics support for the dipole ordering within certain temperature interval [2]. We extended our consideration for the ammonia molecules encapsulated into the same nanotube [3]. Furthermore, we have included into consideration an external electric field to discuss the dielectric properties of the system at hand [4].

1. X. Ma *et al.*, Phys. Rev. Lett. **118**, 027402 (2017).
2. M. Druchok *et al.*, J. Chem. Phys. **158**, 104304 (2023).
3. M. Druchok *et al.*, J. Mol. Liq. **387**, 122633 (2023).
4. P. Sapriianchuk *et al.*, in preparation.

### Beyond the $\epsilon$-expansion: reliable critical exponents in structurally-disordered long-range interacting systems

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We study the impact of weak structural disorder on the critical behavior of spin systems with long-range, power-law decaying interactions [1]. Using field-theoretical renormalization group methods, we analyze the critical properties of the weakly diluted $n$-vector model with long-range interactions in $d$-dimensional space [2]. Our interest here is the stability boundary of the disorder-induced universality class and the correlation length critical exponent $\nu$. By working directly at a fixed spatial dimension ($d = 3$) [3] and employing asymptotic series resummation techniques, we provide more reliable estimates beyond the conventional $\epsilon$-expansion approach [4].

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1. *Dynamics and Thermodynamics of Systems with Long-Range Interactions*, edited by T. Dauxois, S. Ruffo, E. Arimondo, M. Wilkens (Springer-Verlag, New York, 2002).
2. Y. Yamazaki, *Physica A* **90** (1978) 547; D. Benedetti, R. Gurau, S. Harribey, K. Suzuki, *J. Phys. A* **53** (2020) 445008.
3. G. Parisi, *J. Stat. Phys.* **23** (1980) 49; Yu. Holovatch and M. Shpot, *J. Stat. Phys.* **66** (1992) 867.
4. D. Shapoval, M. Dudka, Yu. Holovatch, *Low Temp. Phys.* **48** (2022) 1049; M. Dudka, D. Shapoval, Yu. Holovatch, *J. Phys. Stud.* **28**(2) (2024) 2601.

**Method of canonical transformations in the theory of quantum gases interacting with radiation**

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An approach to the theoretical study of effects and phenomena in quantum gases interacting with radiation is proposed. The approach is based on a modification of the canonical transformation method, which was once used to diagonalize Hamiltonians describing the interaction of electrons with phonons in a solid. The capabilities of the method are demonstrated by studying the influence of photons on the spectral characteristics of atoms of quantum gases interacting with radiation. Within the framework of the developed approach, the effect of "dressing" atoms of quantum gases by a cloud of virtual photons is investigated and expressions for the energy characteristics of such dressed atoms — quasiparticles are obtained. The problem of defining the concept of the effective mass of such quasiparticles is discussed.

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